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Thermodynamic Properties of Elements and Oxides

By L. B. Pankratz

With a section on Process Applications by R.V. Mrazek

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Thermodynamic data on the elements and oxides were reviewed, evaluated, and compiled at the Bureau of Mines Albany Research Center. Values for $C_p°$, $S°$, $H° - H°_{298}$, $-(G° - H°_{298}) / T$, $\Delta Hf°$, $\Delta Gf°$, and log K are given in tabular form. $C_p°$, $H° - H°_{298}$, $\Delta Hf°$, and $\Delta Gf°$ are also expressed algebraically. Examples of calculations using these data are given. A short statement of some fundamental ideas of thermodynamics and several examples of their use are included. The examples illustrate several alternate methods of calculation using both the tabulated values and the equations. Comparisons are also made on the bases of ease of calculation and accuracy of results.

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CONTENTS

METHODS, CONVENTIONS, AND SYMBOLS

The values in this compilation are the result of a review and critical evaluation of relevant thermodynamic data through 1979 for the elements and oxides. Some data published in 1980 have been included. Generally, unless more recent and reliable data were available for the elements, the values given by Hultgren and coworkers were adopted. Similarly, the values for the standard enthalpy of formation at 298.15 K were taken from the NBS Technical Note 270 series. The values for many gases were taken from the JANAF Thermochemical Tables, and those for the actinide elements were taken from the International Atomic Energy Agency publication by Oetting, Rand, and Ackermann. Specific references are made to these publications where they are used.

The selected experimental data were fit with a polynomial in terms of temperature by using a modified form of the computer program described by Justice (*108*).[2] This program, along with a plot of the function $(H^\circ - H^\circ_{298})/T - 298.15$, which must take the value of C_p° at 298.15 K, was used to smoothly merge high-temperature data with low-temperature heat capacity data. The resulting polynomial was then used in a subroutine of the program to calculate standard heat capacities, relative enthalpies, Gibbs energy functions, and standard entropies at selected temperatures. These values are also tabulated at transformation temperatures. In addition, the tables for the oxides include values for the standard enthalpy of formation, Gibbs energy of formation, and logarithm of the equilibrium constant of formation.

Tabulated values and the equations are for the substances in their standard states (indicated by the superscript °). Standard states, for the pure condensed substances, are the most stable form at 1 atm pressure at the specified temperature. For vitreous and metastable substances the superscript refers to the pure substance. For gases, the standard state is the pure substance as a hypothetical ideal gas at unit fugacity.

Tabular values of relative enthalpies are represented by algebraic equations in the form recommended by Maier and Kelley (*151*). This form was fit to the data by Kelley's method (*119*). *Since they consist of no more than four terms, they give less precise values than the tabular values.* However, they do furnish a convenient means of representation. These equations are given below each table. A separate equation is given whenever a transformation occurs. In some cases two equations are used to represent a single phase with an extended temperature range, e. g., carbon and oxygen, since a single equation would give unacceptable errors.

The equations for standard heat capacity, enthalpy of formation, and Gibbs energy of formation are also given below the tables. Since these equations were derived using the equations for standard relative enthalpies, they too give less precise values than the tabular values. Examples 4 and 8 in the applications section show the methods of derivation.

Sources of data used in this compilation are given in the bibliography, which is not meant to be exhaustive. For simplicity, additional sources reviewed but considered less reliable were not included. Estimates were used where the necessary data were lacking. Estimated and extrapolated values are indicated in the tables with an asterisk (*) and a note immediately below the table. An asterisk and a note are also used to indicate decomposition, metastable phases, and irreversible transformations.

The common practice of tabulating five- and sometimes six-digit values has been followed. For example, enthalpy values are given to the nearest calorie. The number of digits given is not intended to reflect the accuracy of the experimental values used. It is an effort to produce internal consistency in the tabulated values.

The following is a list of symbols and constants used:

°	Standard state
T	Thermodynamic temperature in kelvins
K	Kelvin, the unit of thermodynamic temperature.
C_p	Heat capacity at constant pressure.
S	Entropy.
$H - H_{298}$	Enthalpy increment between T and 298.15 K.
$(G - H_{298})/T$	Gibbs energy function, $[(H - H_{298})/T] - S$.
ΔH	Enthalpy change (ΔH_f = enthalpy of formation).
ΔG	Gibbs energy change (ΔG_f = Gibbs energy of formation).
log K	Logarithm (base 10) of the equilibrium constant (log K_f = equilibrium constant of formation).
cal	Thermochemical calorie, 1 cal = 4.1840 joules.
mol	Mole, gram formula weight or molar mass.
ln	Natural logarithm, base e = 2.7183.
P	Pressure in atmosphere, 1 atm = 101.325 kPa.
R	Gas constant, 1.98719 cal/K·mol.
F	Farady constant, 23060.9 cal/volt—equivalent.

[2] Underlined numbers in parentheses refer to items in the list of references at the end of the report.

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THERMODYNAMIC PROPERTIES OF ELEMENTS AND OXIDES

By L. B. Pankratz[1]

With a section on Process Applications by R. V. Mrazek

ABSTRACT

Thermodynamic data on the elements and oxides were reviewed, evaluated, and compiled at the Bureau of Mines Albany Research Center. Values for $C_p°$, $S°$, $H° - H°_{298}$, $-(G° - H°_{298})/T$, $\Delta Hf°$, $\Delta Gf°$, and log K are given in tabular form. $C_p°$, $H° - H°_{298}$, $\Delta Hf°$, and $\Delta Gf°$ are also expressed algebraically. Examples of calculations using these data are given.

INTRODUCTION

This compilation is the first in a series revising and expanding Bureau of Mines Bulletin 605, "Thermodynamic Properties of 65 Elements—Their Oxides, Halides, Carbides, and Nitrides," by C. E. Wicks and F. E. Block, published in 1963, and including data available through 1959. It is part of the Bureau of Mines' continuing effort to provide information for use as guidelines in mineral technology advancement, pollution control, and energy economy.

Wicks and Block prepared their bulletin ". . . to encourage the application of thermodynamics in the metallurgical field; consequently, the values have been presented in a simple, readily usable form." This compilation has been prepared in the same spirit. The values for heat capacities, $C_p°$; high-temperature relative enthalpies, $H° - H°_{298}$; enthalpies of formation, $\Delta H_f°$; and Gibbs energies of formation, $\Delta G_f°$ are given in both tabular and equation form. The tables include Gibbs energy functions $-(G° - H°_{298})/T$, and logarithms (base 10) of the equilibrium constants, log K_f.

Where possible, all phases of an element or oxide are presented in a single table. Temperatures of the transformations and thermodynamic properties at these temperatures are included in the table. Immediately below the table the nature of the transformations is given along with their associated enthalpies.

A short statement of some fundamental ideas of thermodynamics and several examples of their use are included. This section, written by R. V. Mrazek, precedes the tables. The examples illustrate several alternate methods of calculation using both the tabulated values and the equations. Comparisons are also made on the bases of ease of calculation and accuracy of results.

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PROCESS APPLICATIONS

By R. V. Mrazek[1]

The following discussion is intended only to remind the reader of the basic ideas of thermodynamics. These principles will not be developed, nor will required mathematical expressions be derived. For the necessary thorough treatment of both chemical and engineering thermodynamics, the reader is referred to standard textbooks such as those by Lewis and Randall (145), Smith and Van Ness (206), and Van Wylen and Sonntag (231). The emphasis here will be on providing the reader with examples of typical uses for the data presented in this compilation.

First Law of Thermodynamics

The first law of thermodynamics, or energy balance, is perhaps one of the most useful ideas for the practicing scientist or engineer. In applying the first law, attention must be focused upon either a fixed mass (system or closed system) or a particular region in space (open system or control volume). The system is delineated by enclosing it in a boundary. Any region or mass not enclosed by the boundary is usually termed the surroundings.

The first law can be stated in a very general form. However, most common applications will fall into one of two classes, and only the special forms for these classes will be given here. The first is the closed system. Here, attention is focused on some specified mass and a boundary is drawn to enclose only that mass. The primary feature of the closed system is really the nature of its boundary. There can be no mass flux across the boundary; only energy fluxes are allowed. For this case, the first law of thermodynamics takes the standard form

$$\Delta U + mg\Delta Z + m\Delta(V^2/2) = Q - W, \qquad (1)$$

where U = total internal energy of the system,
m = mass of the system,
g = gravitational constant,
Z = height above a reference plane,
V = velocity of the system as a whole,
Q = heat; positive for energy entering the system,
and W = work; positive for energy leaving the system.

The symbol delta, Δ, indicates a difference between the final and initial conditions of the system. For the process being considered, the term ΔU represents the change in internal energy, $mg\Delta Z$ represents the change in potential energy, and $m\Delta(V^2/2)$ represents the change in kinetic energy for the system. Both heat and work have been assigned an arbitrary sign convention. The convention used here is the typical one used in engineering work: energy entering the system as heat is positive, while energy entering the system as work is negative. Heat and work both represent an energy flux crossing the system boundary, so that the first law for a closed system simply states that the change in the total energy contained by a system is equal to the net energy crossing the boundary.

The second, and perhaps more common case considered here is the so-called steady-flow process (an open system). Typically this case is encountered for any

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continuous process where the conditions are not changing with time. A boundary is drawn around a piece of equipment, such as a pump, compressor, furnace, etc. Again the primary features of the steady-flow process are associated with the boundary. The amount of material enclosed by the boundary and the thermodynamic properties of that material are not changing with time. In addition, mass is allowed to cross the boundary, and thus energy enters and leaves this open system (or control volume) not only as heat and/or work, but also because of the energy contained by the mass crossing the boundary. The mass fluxes are constant, and the properties associated with any inlet or exit mass fluxes do not vary with time. For this case, the first law can be written

$$Q - W_x = \Sigma[(h_e + gZ_e + V_e^2/2)m_e] - \Sigma[(h_i + gZ_i + V_i^2/2)m_i], \qquad (2)$$

where W_x = work associated with some kind of machine,
h = specific enthalpy, $u + Pv$,
P = pressure,
u = specific internal energy,
v = specific volume,
e = subscript indicating an exit stream,
i = subscript indicating an inlet stream,

and the other terms and sign conventions are the same as those for the closed system. A delta (Δ) notation is frequently used to represent the summation for all exit streams minus the summation for all inlet streams. The terms for kinetic and potential energy often are not required. If these terms are deleted, the simplified expression then becomes

$$Q - W_x = \Delta(mh), \qquad (3)$$

where (mh) can also be abbreviated as (H), total enthalpy. These expressions simply state that for a steady-flow process, the net boundary flux of energy is zero.

Second Law of Thermodynamics

While the first law of thermodynamics allows the completion of an energy balance for a particular process, it does not place any restrictions on the direction in which the process can proceed, or for that matter, on whether the process can occur at all. These restrictions are stated in the second law of thermodynamics, which can be given for the general case by

$$\Delta S(\text{system}) + \Delta S(\text{surroundings}) \geq 0, \qquad (4)$$

where S represents entropy. (Again, the reader should refer to a standard textbook for a discussion of entropy.) This equation states that, for any process, the total entropy change associated with that process must be greater than or equal to zero. The term $\Delta S(\text{system})$ represents the entropy change that occurs within the system boundary. The term $\Delta S(\text{surroundings})$ represents the entropy change in the surroundings caused by interaction with the system. The equality applies to a reversible process; i.e., a process for which both the system and the surroundings can be returned to their initial conditions. The greater-than sign applies to any real process. There are two restrictions on this equation: First, it applies only to systems that contain a large enough number of particles that the laws of probability hold; second, it cannot be applied to a system (if one exists) where a con-

scious choice can be made on a molecular scale. Thus, it is the form of the second law generally applied to macroscopic systems; i.e., to most processes of engineering interest.

The second law can be applied in several ways, but two applications are most common. Since a reversible process represents the best possible case, the performance of a reversible process can be calculated by setting the total entropy change to zero. These results could then be compared with those for the actual process to determine an efficiency, i.e., how closely the actual process approaches reversibility, or a quantitative measure of the efficiency of energy utilization. The second common method of applying the second law allows the determination of whether a proposed process is even possible. Here, one would calculate the total entropy change associated with the proposed process, and from this value, judge the process. If the total entropy change is negative, the process is not possible. If the total entropy change is zero, indicating a reversible process, one must also conclude that the process is not really possible, since reversibility is a theoretical optimum. Thus, any possible process will be associated with a positive total entropy change.

Equilibrium

In addition to the first law of thermodynamics, the practicing scientist and engineer are frequently interested in equilibrium in reacting systems. While this topic could be treated in terms of entropy, or the second law of thermodynamics, it is more frequently (and conveniently) treated in terms of the Gibbs energy, G, where

$$G = H - TS. \tag{5}$$

For a general reaction such as

$$bB + cC = \ell L + mM, \tag{6}$$

where capital letters represent chemical species and lowercase letters represent mole numbers in the balanced reaction, the state of equilibrium can be represented by the expressions

$$\Delta G^\circ = -RT \ln Ka \tag{7}$$

and

$$Ka = a_L^{\ell} a_M^{m} / a_B^{b} a_C^{c}. \tag{8}$$

In these expressions, the superscript (°) represents the standard state so that ΔG° is the change in the Gibbs energy that occurs when "b" moles of B and "c" moles of C, in their standard states, react to form "ℓ" moles of L and "m" moles of M, in their standard states. Other symbols are defined as

Ka = equilibrium constant, defined by equation 8,
a = activity, the ratio of fugacity to standard-state fugacity,
T = thermodynamic temperature,
and
R = universal gas constant.

To use these expressions effectively, a value of the standard-state change in the Gibbs function, ΔG°, is needed. This can be calculated from the values in this compilation. In addition, the activity of each species in the system must be rep-

resented as a function of temperature, pressure, and composition. If this can be done, the conditions of equilibrium for a reaction or set of reactions can be calculated from the expressions for the equilibrium constants for the reactions, Ka, stoichiometry, and other restrictions on the system such as the first law of thermodynamics. Before undertaking such calculations, the user should be sure that the proper number of reactions for a particular process is being considered; see, for example, Smith and Van Ness (206, pp. 415-418).

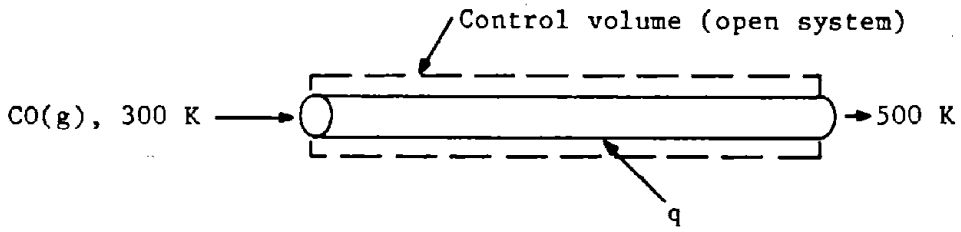
Examples

The previous discussion was deliberately brief. The application of these basic ideas is illustrated in the following examples. Where several methods of doing a particular calculation are given, comparisons based on ease of use and accuracy of the results are also given.

Example 1

A stream of carbon monoxide is heated in a steady-flow process from 300 to 500 K at 1 atm. Calculate the required energy input (as heat) per mole of carbon monoxide.

All of the possible methods of treating this calculation are based on the steady-flow form of the first law of thermodynamics, reduced for this particular case as follows:



$$q - \cancel{w_x}^{\,0} = \Delta H$$

For any method chosen, it is necessary to calculate the enthalpy change for the carbon monoxide. At this pressure, ideal gases may be assumed.

Method 1

The easiest and most accurate procedure is to use the tabulated values of $H^\circ_T - H^\circ_{298}$. From the table for CO(g),

$$H^\circ_{300} - H^\circ_{298} = 13 \text{ cal/mol},$$

$$H^\circ_{500} - H^\circ_{298} = 1417 \text{ cal/mol},$$

$$q = H^\circ_{500} - H^\circ_{300} = (H^\circ_{500} - H^\circ_{298}) - (H^\circ_{300} - H^\circ_{298}),$$

and

$$q = 1417 - 13 = 1404 \text{ cal/mol CO(g)}.$$

The positive sign indicates an input of energy as heat.

Method 2

If many such calulations are to be made, it might be more convenient to express $H_T^\circ - H_{298}^\circ$ in the form of an equation, rather than as tabulated values. For CO(g) the equation given for $H_T^\circ - H_{298}^\circ$ (cal/mol) is

$$H_T^\circ - H_{298}^\circ = 6.708\ T + 0.553\times10^{-3}T^2 + 6.20\times10^3/T - 2070.$$

This equation will give, rounded to the nearest calorie,

$$H_{300}^\circ - H_{298}^\circ = 13 \text{ cal/mol},$$

$$H_{500}^\circ - H_{298}^\circ = 1435 \text{ cal/mol},$$

and $$q = (H_{500}^\circ - H_{298}^\circ) - (H_{300}^\circ - H_{298}^\circ) = 1422 \text{ cal/mol}.$$

This differs from the more accurate answer calculated in method 1 by 18 cal/mol, or approximately 1.3 pct. Small differences are to be expected, since the equations given are all of the same standard form rather than the equations actually used to generate the tabulated values.

The calculation could equally well be done by using the equation given for Cp° (cal/mol·K):

$$Cp^\circ = 6.708 + 1.106\times10^{-3}T - 6.20\times10^3/T^2,$$

then $$H_{500}^\circ - H_{300}^\circ = \int_{300}^{500} Cp\ dT$$

$$= 6.708(500-300) + 1/2(1.106\times10^{-3})(500^2-300^2) + 6.20\times10^3(1/500-1/300)$$

$$= 1422 \text{ cal/mol·K}.$$

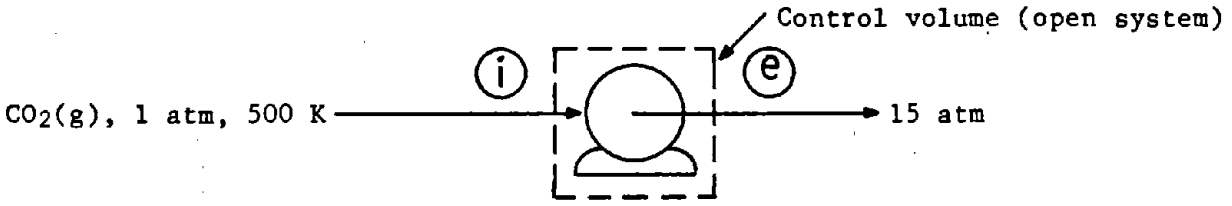
The result is identical to the one obtained above from the equations for $H_T^\circ - H_{298}^\circ$. This must be true, within round-off error in the calculation, because the equations for Cp° were derived from the equations for $H_T^\circ - H_{298}^\circ$.

It should be emphasized here that the tables give best values selected during evaluation of the experimental data. The calculation, as done above in method 1 is both the easiest and the most accurate. The equations for Cp° and $H_T^\circ - H_{298}^\circ$ have been included, not to encourage their use, but rather for the convenience of those who prefer their use and for those doing design calculations by computer. Whenever the equations are used, some sacrifice in accuracy is made compared with using the tabulated values.

Example 2

A stream of carbon dioxide is being compressed adiabatically in a steady-flow process from 1 atm, 500 K to 15 atm. The compressor has an efficiency of 80 pct compared with a reversible machine. Calculate the required energy input (as work) and the temperature of the carbon dioxide leaving the compressor.

Since it already has been noted that the tabulated values are the easiest to use, only those values will be used in this solution. In addition, with the conditions given, carbon dioxide may be considered an ideal gas. The first law of thermodynamics may be reduced for this case as follows:



Compressor

$$\overset{0}{q} - w_x = \Delta H$$

Thus, we need to calculate the enthalpy change for the carbon dioxide. In this case, however, the first law of thermodynamics does not give sufficient information to calculate the desired quantities. Since the exit temperature of the carbon dioxide is unknown, the required enthalpy change cannot be calculated. The required information can, however, be obtained by using the second law and the given efficiency of the compressor.

Consider a compressor that is both adiabatic and reversible. In this case, the second law will reduce to the form

$$S_e = S_i$$

for the carbon dioxide. For an ideal gas,

$$dS = Cp^\circ\ dT/T - R\ dP/P.$$

If this equation is integrated between the inlet and exit states for the compressor, indicated by "i" and "e" on the diagram above,

$$S_e - S_i = \int_{T_i}^{T_{es}} Cp^\circ\ dT/T - R\ \ln(Pe/Pi) = 0,$$

where T_{es} represents the exit temperature for the reversible machine, <u>not</u> the actual process. Then

$$\int_{T_i}^{T_{es}} Cp^\circ\ dT/T = R\ \ln(Pe/Pi).$$

The integral on the left side of this equation can easily be evaluated from the tabulated properties for carbon dioxide, since

$$\int_{T_1}^{T_2} Cp^\circ\ dT/T = S^\circ_{T_2} - S^\circ_{T_1}.$$

Thus $$S^\circ_{Tes} - S^\circ_{Ti} = R \ln(Pe/Pi).$$

For the machine being considered,

$$T_i = 500 \text{ K and } S^\circ_{Ti} = S^\circ_{500} = 56.120 \text{ cal/mol}\cdot\text{K};$$

also $$P_i = 1 \text{ atm and } P_e = 15 \text{ atm.}$$

Substituting gives $$S^\circ_{Tes} - 56.120 = 1.987 \ln(15/1).$$

This can be solved for S°_{Tes}, for which

$$S^\circ_{Tes} = 56.120 + 1.987 \ln 15 = 61.501 \text{ cal/mol}\cdot\text{K}.$$

Interpolation may then be used to obtain T_{es} from the tables, and once T_{es} is obtained, H°_{es} can be found. Remember, however, that T_{es} and H°_{es} do not represent the exit conditions for the actual machine, but rather the exit conditions that would exist if the machine were reversible. The table for carbon dioxide gives the following:

T, K	S_T, cal/mol·K	$H^\circ_T - H^\circ_{298}$, cal/mol
700	59.908	4245
800	61.520	5453
900	62.990	6702

Then, by interpolation,

$$T_{es} = 700 + (800-700)[(61.501-59.908)/(61.520-59.908)] = 798.8 \text{ K}$$

and $$H^\circ_{Tes} - H^\circ_{298} = 4245 + (5453-4245)[(798.8-700)/(800-700)] = 5439 \text{ cal/mol.}$$

Also $$H^\circ_{Ti} - H^\circ_{298} = H^\circ_{500} - H^\circ_{298} = 1987 \text{ cal/mol.}$$

For the reversible, adiabatic machine

$$-w_{xs} = H^\circ_{Tes} - H^\circ_{Ti} = (H^\circ_{Tes} - H^\circ_{298}) - (H^\circ_{Ti} - H^\circ_{298})$$
$$= 5439 - 1987 = 3452 \text{ cal/mol},$$

where the extra subscript "s" on w_x again represents the reversible process. Now, we may use the definition of efficiency, η, for a compressor to determine the work for the actual machine, w_x:

$$\eta = w_{xs}/w_x$$

or $$w_x = w_{xs}/\eta = -3452/0.80 = -4315 \text{ cal/mol.}$$

The first law of thermodynamics for the actual machine is

$$-w_x = H_{Te} - H_{Ti} = (H^\circ_{Te} - H^\circ_{298}) - (H^\circ_{Ti} - H^\circ_{298}),$$

where Te is the actual exit temperature. We now have

$$-(-4315) = (H^\circ_{Te} - H^\circ_{298}) - (1987)$$

or $$H^\circ_{Te} - H^\circ_{298} = 6302 \text{ cal/mol.}$$

Again, interpolation allows us to determine Te.

$$Te = 800 + (900-800)\,[(6302-5453)/(6702-5453)] = 868 \text{ K.}$$

Note that Te is significantly higher than T_{es}. We now have determined that the temperature of the carbon dioxide at the compressor exit is 868 K and the required energy input (as work) to the actual compressor is 4315 cal/mol of CO_2.

Example 3

One of the reactions involved in the production of molybdenum metal is a simple hydrogen reduction:

$$MoO_2(c) + 2H_2(g) = Mo(c) + 2\,H_2O(g).$$

Calculate the standard enthalpy change, ΔH°_{298}, for this reaction at 298 K.

The desired result can be calculated directly from the standard enthalpies of formation for the substances involved.

$$\Delta Hf^\circ_{298} = \underset{\text{product}}{\Sigma \nu_i \Delta Hf^\circ_{i\,298}} - \underset{\text{reactant}}{\Sigma \nu_i \Delta Hf^\circ_{i\,298}},$$

where ΔHf°_i = enthalpy change of formation of species i,

and ν_i = mole number of species i in the balanced reaction.

For this reaction, $\nu_{MoO_2} = 1$, $\nu_{Mo} = 1$,

$\nu_{H_2} = 2$, $\nu_{H_2O} = 2$,

and $\Delta H^\circ_{298} = \Delta Hf^\circ_{Mo(c)_{298}} + 2\Delta Hf^\circ_{H_2O(g)_{298}} - 2\Delta Hf^\circ_{H_2(g)_{298}} - \Delta Hf^\circ_{MoO_2(g)_{298}}$.

From the tables, at 298 K, $\Delta Hf^\circ_{Mo(c)} = 0$ cal/mol,

$\Delta Hf^\circ_{H_2O(g)} = -57795$ cal/mol,

$\Delta Hf^\circ_{H_2(g)} = 0$ cal/mol,

and $\Delta Hf^\circ_{MoO_2(c)} = -140760$ cal/mol.

Thus $$H^\circ_{298} = 2(-57795) - 1(-140760) = 25170 \text{ cal.}$$

Example 4

The actual temperature at which the reaction of example 3 is carried out is approximately 1300 K. Calculate the standard enthalpy change for the reaction at this temperature, ΔH°_{1300}.

Method 1

The easiest way to do this calculation is to use the method shown in example 3, but for 1300 K. Thus,

$$\Delta H^\circ_{1300} = \Delta Hf^\circ_{Mo(c)_{1300}} + 2\Delta Hf^\circ_{H_2O(g)_{1300}} - 2\Delta Hf^\circ_{H_2(g)_{1300}} - \Delta Hf^\circ_{MoO_2(c)_{1300}},$$

and from the tables, $\Delta Hf^\circ_{Mo(c)_{1300}} = 0$ cal/mol,

$\Delta Hf^\circ_{H_2O(g)_{1300}} = -59632$ cal/mol,

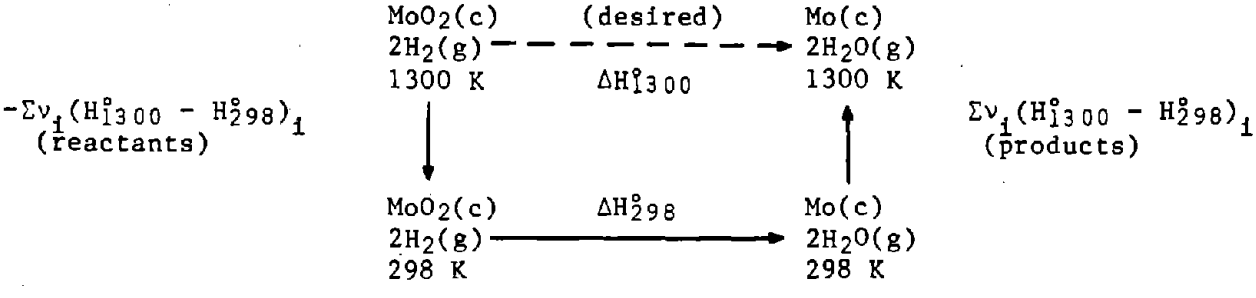
$\Delta Hf^\circ_{H_2(g)_{1300}} = 0$ cal/mol,

and $\Delta Hf^\circ_{MoO_2(c)_{1300}} = -137139$ cal/mol.

So $\Delta H^\circ_{1300} = 2(-59632) - 1(-137139) = 17875$ cal.

Method 2

This calculation can also be done using the value of ΔH°_{298} calculated in example 3 and the tabulated values of $H^\circ_T - H^\circ_{298}$ for each of the four species. It is possible to do this because we are calculating the change in a property, in this case enthalpy, and the thermodynamic properties are independent of the path by definition. Thus, we may use any path for our calculation; e.g., the one shown below:



The enthalpy changes for each process along our path are shown in the diagram. This path corresponds to cooling the reactants from 1300 K to 298 K, reacting them at 298 K, and heating the products back up to 1300 K. Thus,

$$\Delta H^\circ_{1300} = \underset{\text{products}}{\Sigma\nu_i(H^\circ_{1300} - H^\circ_{298})_i} + \Delta H^\circ_{298} - \underset{\text{reactants}}{\Sigma\nu_i(H^\circ_{1300} - H^\circ_{298})_i}.$$

For our reaction, the values of ν_i and ΔH°_{298} are given in example 3, and from the tables,

$(H^\circ_{1300} - H^\circ_{298})_{Mo(c)} = 6542$ cal/mol,

$(H^\circ_{1300} - H^\circ_{298})_{H_2O(g)} = 9298$ cal/mol,

$(H^\circ_{1300} - H^\circ_{298})_{H_2(g)} = 7151$ cal/mol,

and $(H^\circ_{1300} - H^\circ_{298})_{MoO_2(c)} = 18132$ cal/mol.

Then $$\Delta H^\circ_{1300} = (H^\circ_{1300} - H^\circ_{298})_{Mo(c)} + 2(H^\circ_{1300} - H^\circ_{298})_{H_2O(g)} + \Delta H^\circ_{298} - (H^\circ_{1300} - H^\circ_{298})_{MoO_2(c)} - 2(H^\circ_{1300} - H^\circ_{298})_{H_2(g)}$$

$$= 6542 + 2(9298) + 25170 - (18132) - 2(7151)$$

$$= 17874 \text{ cal.}$$

This result is the same as that calculated by method 1, within 1 cal. This small difference is the result of round-off error in the tabulated values.

Method 3

If this calculation were to be done by computer, or for many different temperatures, it is more convenient to have an equation for ΔH°_T. To derive this equation is straightforward as long as all of the heat capacity equations are of the same form. For the standard form adopted here,

$$Cp = a + bT + c/T^2,$$

the equation for ΔH°_T will have the form (145, p. 72)

$$\Delta H^\circ_T = \Delta H^\circ_o + \Delta a\, T + \Delta b T^2/2 - \Delta c/T,$$

where ΔH°_o is a constant to be determined from a known value of ΔH°_T at one temperature, and Δa, Δb, and Δc are calculated from the Cp° equations; e.g.,

$$\Delta a = \underset{\text{product}}{\Sigma \nu_i a_i} - \underset{\text{reactant}}{\Sigma \nu_i a_i}.$$

Thus for our reaction

$$\Delta a = a_{Mo(c)} + 2a_{H_2O(g)} - a_{MoO_2(c)} - 2a_{H_2(g)}$$

$$= 4.377 + 2(6.895) - 14.786 - 2(6.456)$$

$$= -9.531.$$

The calculation of Δa, Δb, and Δc is most easily done in tabular form, as follows:

	a	b x 10^3	c x 10^{-3}
Mo(c)	4.377	2.370	59.20
$H_2O(g)$	6.895	2.882	24.00
$MoO_2(c)$	14.786	4.982	-257.00
$H_2(g)$	6.456	.838	16.50
Δ	-9.531	1.476	331.20

Then $$\Delta H^\circ_T = \Delta H^\circ_o - 9.531\, T + 1.476\times10^{-3} T^2/2 - 331.20\times10^3/T.$$

We also know $\Delta H^\circ_{298} = 25170$ cal from example 3. This can be substituted into the equation above to give

$$25170 = \Delta H^\circ_o - 9.531(298.15) + 0.738\times10^{-3}(298.15)^2 - 331.20\times10^3/298.15.$$

This last expression can be solved for

$$\Delta H^\circ_o = 29057 \text{ cal},$$

and $$\Delta H^\circ_T = 29057 - 9.531\ T + 0.738\times10^{-3}T^2 - 331.20\times10^3/T.$$

This expression can be used to calculate ΔH°_T at any desired temperature within the range of validity of the equations for Cp°. If we use it to calculate ΔH°_{300}, the result is

$$\Delta H^\circ_{300} = 17659 \text{ cal}.$$

This differs from the more accurate answer calculated in method 1 by 216 cal, or about 1.2 pct. As seen in example 1, these differences are to be expected since we are using standard-form equations rather than the tabular data.

Method 4

The equation for ΔH°_T may also be derived by using the equations for $H^\circ_T - H^\circ_{298}$ and the known values for ΔH°_{298}. This is analogous to using method 2, except equations for $H^\circ_T - H^\circ_{298}$ are used rather than the tabulated values. The desired expression for ΔH°_T is

$$\begin{aligned}\Delta H^\circ_T &= H^\circ_{T[Mo(c)]} + 2H^\circ_{T[H_2O(g)]} - 2H^\circ_{T[H_2(g)]} - H^\circ_{T[MoO_2(c)]} \\ &= (H^\circ_T - H^\circ_{298})_{Mo(c)} + 2(H^\circ_T - H^\circ_{298})_{H_2O(g)} - 2(H^\circ_T - H^\circ_{298})_{H_2(g)} \\ &\quad - (H^\circ_T - H^\circ_{298})_{MoO_2(c)} + [H^\circ_{298_{Mo(c)}} + 2H^\circ_{298_{H_2O(g)}} - 2H^\circ_{298_{H_2(g)}} \\ &\quad - H^\circ_{298_{MoO_2(c)}}].\end{aligned}$$

Note that the term in brackets is ΔH°_{298}, which is 25170 cal from example 3. The equations for $H^\circ_T - H^\circ_{298}$ are found in the tables (in cal/mol):

$$(H^\circ_T - H^\circ_{298})_{Mo(c)} = 4.377\ T + 1.185\times10^{-3}T^2 - 59.20\times10^3/T - 1212,$$

$$(H^\circ_T - H^\circ_{298})_{H_2O(g)} = 6.895\ T + 1.441\times10^{-3}T^2 - 24.00\times10^3/T - 2103,$$

$$(H^\circ_T - H^\circ_{298})_{H_2(g)} = 6.456\ T + 0.419\times10^{-3}T^2 - 16.50\times10^3/T - 1907,$$

and $$(H^\circ_T - H^\circ_{298})_{MoO_2(c)} = 14.786\ T + 2.491\times10^{-3}T^2 + 257.00\times10^3/T - 5492.$$

$$\begin{aligned}\text{So } \Delta H^\circ_T &= [4.377 + 2(6.895) - 2(6.456) - 14.786]T + [1.185 + 2(1.441) - 2(0.419) \\ &\quad - 2.491]\times10^{-3}T^2 + [(-59.20) + 2(-24.00) - 2(-16.50) - 257.00]\times10^3/T \\ &\quad + [(-1212) + 2(-2103) - 2(-1907) - (-5492)] + 25170;\end{aligned}$$

$$\Delta H^\circ_T = 29058 - 9.531\ T + 0.738\times10^{-3}T^2 - 331.20\times10^3/T.$$

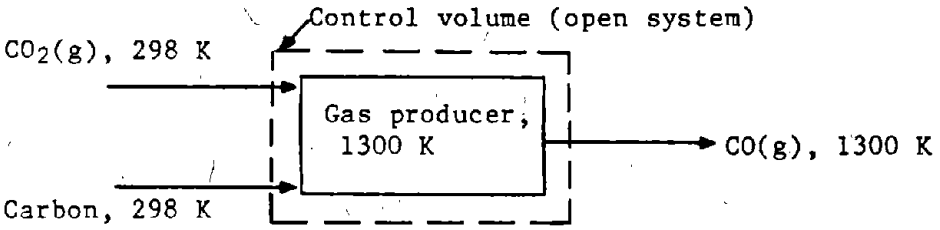
Comparison of this equation with the result of method 3 shows that they are the

same within 1 cal in the first term on the right side of the equation.

Again, the preferred and most accurate calculation is that shown in method 1. However, those methods that generate an equation for ΔH°_T as a function of temperature may be preferable for those doing computer work.

Example 5

Carbon monoxide for use as a reducing gas is to be generated by reacting a stream of carbon dioxide with pure carbon in a flow process at 1 atm. Although coke would be used in an industrial gas producer, carbon will be considered to be graphite for the purposes of this example. The gas producer will operate continuously at 1300 K, and it will be assumed that equilibrium conditions will prevail at the exit. Under these conditions, as will be shown in a subsequent example, this corresponds to very nearly 100-pct conversion to carbon monoxide. The process can be depicted as follows:



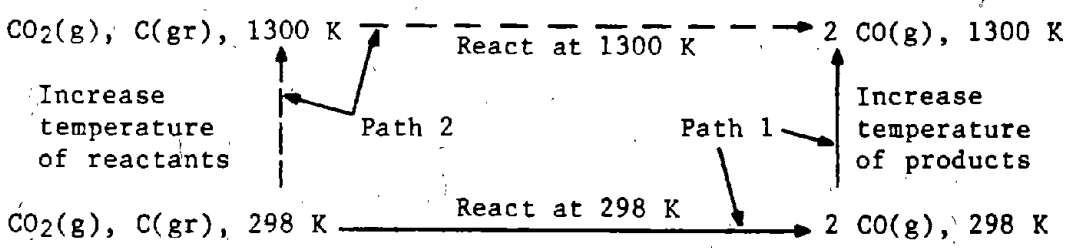
$$CO_2(g) + C(gr) = 2\ CO(g)$$

Determine the minimum amount of energy that must be added to the process (as heat, in this case) per mol of $CO_2(g)$ feed.

The first law of thermodynamics can be reduced for this case to

$$q - \cancel{w_x}^{\,0} = \Delta H.$$

Once again we need to determine an enthalpy change for the process of interest, and we may again take advantage of the fact that the change in enthalpy is not a function of path. In this case, there are two paths for which the use of tabulated data is probably equally convenient. These are shown in the following diagram:



For path 1, shown above, ΔH may be calculated as

$$\Delta H = 2H_{CO(g)_{1300}} - H_{CO_2(g)_{298}} - H_{C(gr)_{298}},$$

or $$\Delta H = 2(H^\circ_{1300} - H^\circ_{298})_{CO(g)} + [2H^\circ_{CO(g)} - H^\circ_{CO_2(g)} - H^\circ_{C(gr)}]_{298},$$

where the last term on the right is ΔH°_{298} for the reaction. Thus,

$$\Delta H = 2(H^\circ_{1300} - H^\circ_{298})_{CO(g)} + 2\Delta Hf^\circ_{CO(g)_{298}} - \Delta Hf^\circ_{CO_2(g)_{298}}.$$

Each of these terms may be evaluated from the tables:

$$(H^\circ_{1300} - H^\circ_{298})_{CO(g)} = +7616 \text{ cal/mol},$$

$$\Delta Hf^\circ_{CO(g)_{298}} = -26417 \text{ cal/mol},$$

$$\Delta Hf^\circ_{CO_2(g)_{298}} = -94051 \text{ cal/mol},$$

and $\Delta H = q = 2(7616) + 2(-26417) - (-94051) = 56449$ cal/mol of CO_2 fed.

This value represents the minimum energy requirement since any heat losses from the reactor would require the input of additional energy to make up for the losses. Now, the calculation will be repeated for path 2 shown above.

For path 2,

$$\Delta H = 2H^\circ_{CO(g)_{1300}} - H^\circ_{CO_2(g)_{298}} - H^\circ_{C(gr)_{298}}$$

$$= (H^\circ_{1300} - H^\circ_{298})_{CO_2(g)} + (H^\circ_{1300} - H^\circ_{298})_{C(gr)} + [2H^\circ_{CO} - H^\circ_{CO_2} - H^\circ_{C}]_{1300},$$

where the last term in brackets is ΔH°_{1300} for the reaction. Thus,

$$\Delta H = (H^\circ_{1300} - H^\circ_{298})_{CO_2(g)} + (H^\circ_{1300} - H^\circ_{298})_{C(gr)} + 2\Delta Hf^\circ_{CO(g)_{1300}} - \Delta Hf^\circ_{CO_2(g)_{1300}}.$$

The tables give the following:

$$(H^\circ_{1300} - H^\circ_{298})_{CO_2(g)} = +11988 \text{ cal/mol},$$

$$(H^\circ_{1300} - H^\circ_{298})_{C(gr)} = +4431 \text{ cal/mol},$$

$$\Delta Hf^\circ_{CO(g)_{1300}} = -27217 \text{ cal/mol},$$

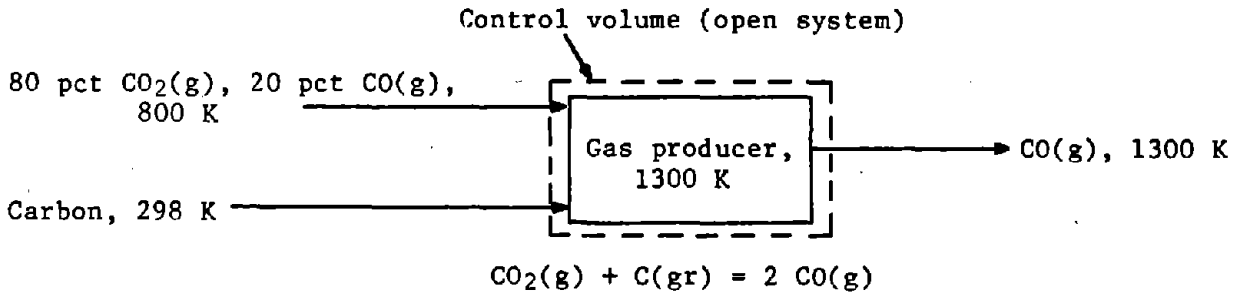
$$\Delta Hf^\circ_{CO_2(g)_{1300}} = -94463 \text{ cal/mol},$$

and $\Delta H = q = 11988 + 4431 + 2(-27217) - (-94463) = 56448$ cal/mol of CO_2 fed.

Note that this differs from the result calculated for path 1 by only 1 cal. Both of these calculations are equally simple and make efficient use of the tabulated data.

Example 6

If the carbon monoxide produced in the process described in example 5 were used as a reducing gas, it would not all be reacted in the reduction process. In this case, the off gas from the reduction process can be recycled through the gas producer. A possible set of conditions is shown in the following diagram:

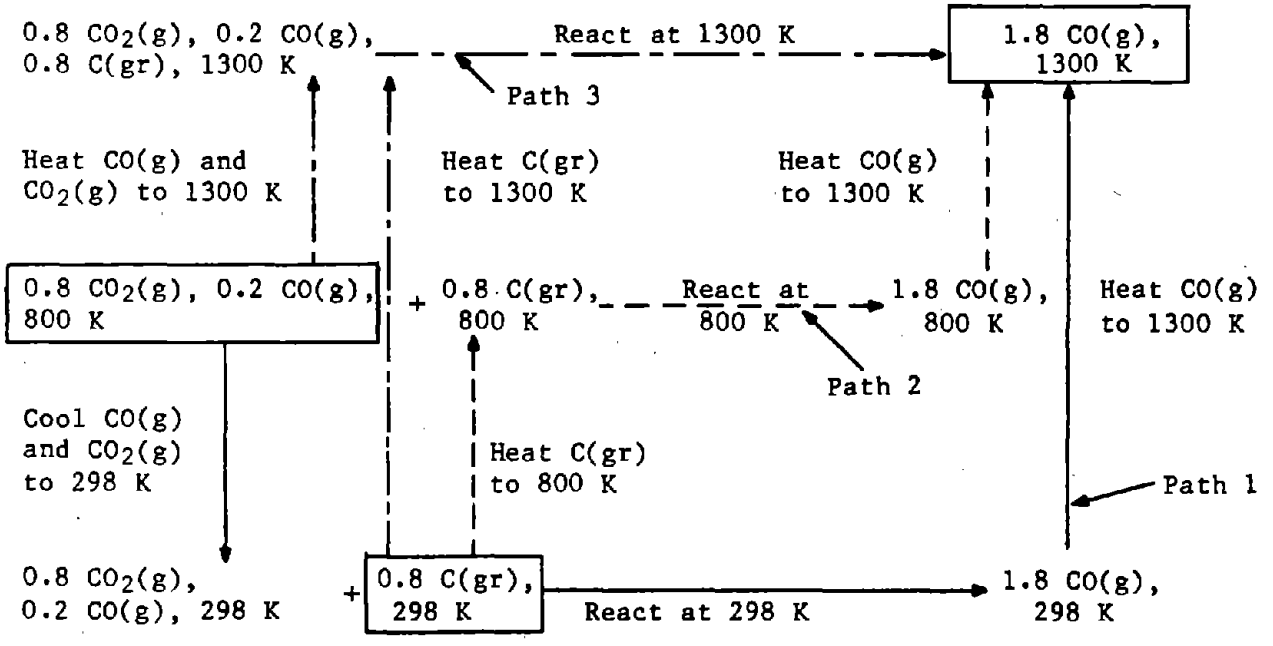


Again, let us calculate the minimum energy requirements, as heat.

The first law of thermodynamics will show that

$$q = \Delta H.$$

For convenience, we will base our calculation on 1 mol of entering gas mixture (80 pct CO_2, 20 pct CO). Note that in this case, there are several convenient paths that may be used for the calculation of the change in enthalpy. Three such possible paths are shown on the following diagram, where, for clarity, the actual reactants at their initial conditions and the product at its final conditions are enclosed in boxes. The other states noted on the diagram are intermediate states for some path being illustrated.



For path 1(———— in diagram),

$$\Delta H = -0.8(H^\circ_{800} - H^\circ_{298})_{CO_2(g)} - 0.2(H^\circ_{800} - H^\circ_{298})_{CO(g)} + 0.8[2\Delta Hf^\circ_{CO(g)} - \Delta Hf^\circ_{CO_2(g)}]_{298} + 1.8(H^\circ_{1300} - H^\circ_{298})_{CO(g)}.$$

For path 2 (— — — —in diagram),

$$\Delta H = 0.8(H^\circ_{800} - H^\circ_{298})_{C(gr)} + 0.8[2\Delta Hf^\circ_{CO(g)} - \Delta Hf^\circ_{CO_2(g)}]_{800}$$

$$+ 1.8[(H^\circ_{1300} - H^\circ_{298})_{CO(g)} - (H^\circ_{800} - H^\circ_{298})_{CO(g)}].$$

For path 3 (——– – ——– in diagram),

$$\Delta H = 0.8[(H^\circ_{1300} - H^\circ_{298})_{CO_2(g)} - (H^\circ_{800} - H^\circ_{298})_{CO_2(g)}] + 0.8(H^\circ_{1300} - H^\circ_{298})_{C(gr)} + 0.2[(H^\circ_{1300} - H^\circ_{298})_{CO(g)} - (H^\circ_{800} - H^\circ_{298})_{CO(g)}] + 0.8[2\Delta Hf^\circ_{CO(g)} - \Delta Hf^\circ_{CO_2(g)}]_{1300}.$$

The required values (cal/mol) can be found in the tables:

	298 K	800 K	1300 K
$\Delta Hf^\circ_{CO(g)}$	-26417	-26507	-27217
$\Delta Hf^\circ_{CO_2(g)}$	-94051	-94208	-94463
$(H^\circ_T - H^\circ_{298})_{CO(g)}$	0	3627	7616
$(H^\circ_T - H^\circ_{298})_{CO_2(g)}$	0	5453	11988
$(H^\circ_T - H^\circ_{298})_{C(gr)}$	0	1825	4431

Thus for path 1,

$$\Delta H_1 = -0.8(5453) - 0.2(3627) + 0.8[2(-26417) - (-94051)] + 1.8(7616)$$

$$= 41595 \text{ cal/mol gas fed.}$$

For path 2,

$$\Delta H_2 = 0.8(1825) + 0.8[2(-26507) - (-94208)] + 1.8(7616-3627)$$

$$= 41595 \text{ cal/mol gas fed.}$$

For path 3,

$$\Delta H_3 = 0.8(11988 - 5453) + 0.8(4431) + 0.2(7616 - 3627) + 0.8[2(-27217) - (-94463)]$$
$$= 41594 \text{ cal/mol gas fed.}$$

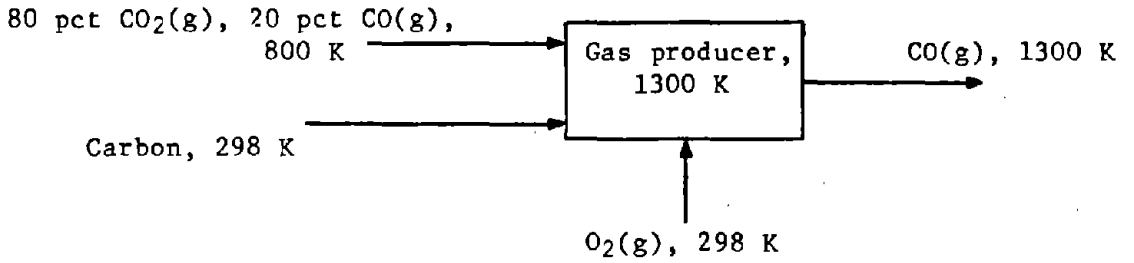
Example 7

One method of providing the energy required by the gas producer in example 6 is to blow enough oxygen into the bed of carbon so that the process is sustained by the energy derived from the reaction

$$C(gr) + 0.5\ O_2(g) = CO(g).$$

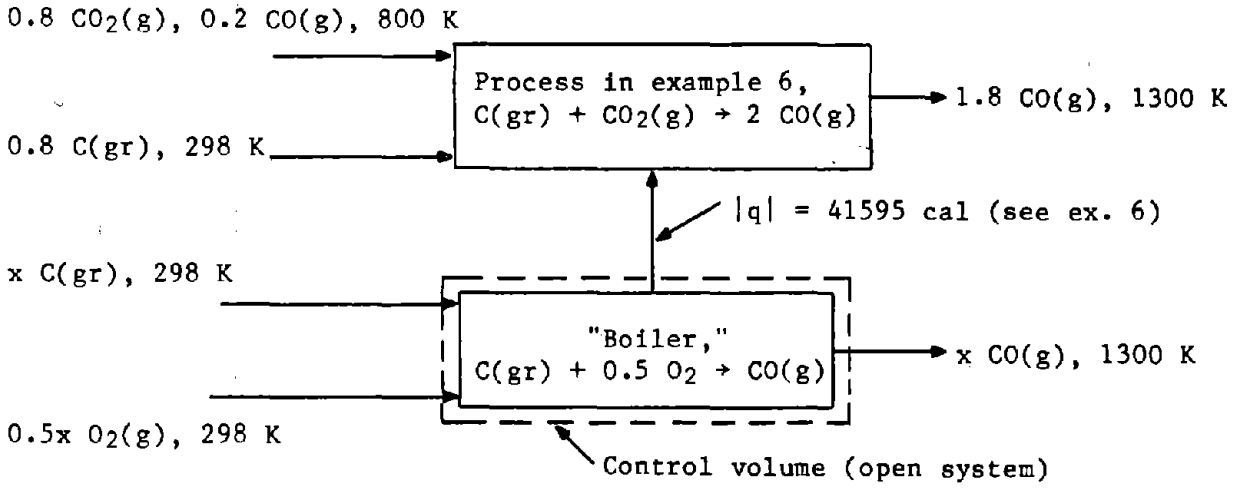
Note that, as will be shown in example 9, very little carbon dioxide will be produced at these conditions. What is the minimum oxygen requirement to sustain the process?

The actual process being considered can be depicted as shown below.



$$CO_2(g) + C(gr) = 2\ CO(g)$$
$$0.5\ O_2(g) + C(gr) = CO(g)$$

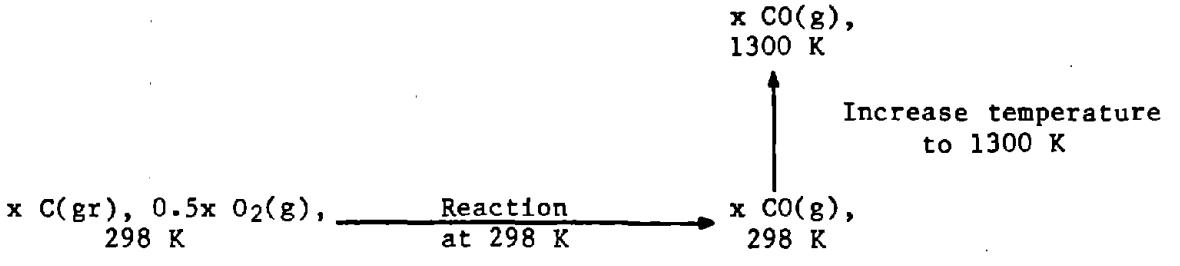
We could analyze this whole process. However, we have already completed the major portion of the analysis (the first reaction) for a feed of 1 mol of CO_2-CO gas into the gas producer. (See example 6.) Thus, it is much easier at this point to visualize the processes being considered here in two parts. This case can be depicted as



In this example, we are interested in the "boiler" shown above. For this system, the first law of thermodynamics is

$$q = \Delta H = -41595 \text{ cal (path 1, example 6)},$$

and we need only to consider the reaction in the "boiler." Therefore, a convenient path for the calculation of the enthalpy change would be combustion at 298 K followed by a temperature change to 1300 K.



Thus, $\Delta H = x[\Delta Hf^\circ_{CO(g)_{298}} + (H^\circ_{1300} - H^\circ_{298})_{CO(g)}] = q = -41595$ cal.

Substituting values from the tables for CO(g) (see also example 6),

$$-41595 = x[-26417 + 7616]$$

$$x = 2.212.$$

Thus, oxygen required = 1.106 mol/mol inlet CO-CO_2 mixture.

Several things should be noted here. First, this represents a minimum oxygen requirement to sustain the process, since any heat losses would have to be balanced by the combustion of more carbon (and thus require more oxygen). Second, the sign on the heat term in the first law expression for the "boiler" is negative because energy is leaving the system as heat, and our sign convention thus dictates the use of the negative sign. Third, the calculations done in examples 6 and 7 were straightforward because of the format of the tables. Last, one should note that breaking the whole process into two separate parts, as in examples 6 and 7, made the required calculations easier.

Example 8

As a simple example dealing with chemical equilibrium and the use of standard-state Gibbs energy, consider the thermal decomposition of silver oxide at 500 K:

$$2\ Ag_2O(c) = 4\ Ag(c) + O_2(g).$$

If the system is at fairly high temperature and low pressure, ideal gas behavior may be assumed. In addition, the solubility of silver oxide in silver at 500 K is very low; thus we may assume that the solids exist as pure substances. Thus, the expression for equilibrium can be written as

$$\Delta G^\circ = -RT\ \ln Ka$$

and

$$Ka = a^4_{Ag(c)} a_{O_2(g)} / a^2_{Ag_2O(c)},$$

where "a" represents the activity. For pure solids at relatively low pressure and a standard state of the pure substance at 1 atm, the activity of the solid may be approximated as

$$a_{solid} \simeq 1.$$

If, in addition, ideal gas behavior is assumed, for a standard state of the pure ideal gas at a pressure of 1 atm, the activity of oxygen can be evaluated as

$$a_{O_2(g)} = \overline{P}_{O_2},$$

where $\overline{P}_{O_2}$ is the partial pressure of oxygen (atm) in the system at equilibrium. For this case, where oxygen is the only gaseous species present, this becomes

$$\overline{P}_{O_2} = P, \text{ the system pressure in atm.}$$

Thus for the reaction of interest,

$$Ka = P$$

and $$P = \exp(-\Delta G^\circ_T/RT).$$

The decomposition pressure for silver oxide, P, can then be determined by evaluating the standard-state change in the Gibbs energy for the decomposition reaction at the temperature of interest. This can be done from the information in the tables in several ways. Again, several methods of calculation will be illustrated.

Method 1

The most straightforward method of calculation relies on the use of the tabulated values of ΔGf°_T, the standard-state change in the Gibbs energy for formation reactions. Here again, as with enthalpy changes (see example 3), ΔG°_T for the reaction of interest can be found from

$$\Delta G^\circ_T = \underset{\text{products}}{\Sigma \nu_i \Delta Gf^\circ_T} - \underset{\text{reactants}}{\Sigma \nu_i \Delta Gf^\circ_T}.$$

For the reaction of interest,

$$\nu_{O_2(g)} = 1,$$

$$\nu_{Ag(c)} = 4,$$

$$\nu_{Ag_2O(c)} = 2,$$

and from the tables for 500 K,

$$\left.\begin{aligned} \Delta Gf^\circ_{O_2(g)} &= 0 \text{ cal/mol}, \\ \Delta Gf^\circ_{Ag(c)} &= 0 \text{ cal/mol}, \\ \text{and} \quad \Delta Gf^\circ_{Ag_2O(c)} &= 445 \text{ cal/mol}. \end{aligned}\right\} \text{ at 500 K}$$

Thus, for this reaction,

$$\Delta G^\circ_{500} = -2\Delta Gf^\circ_{Ag_2O(c)_{500}} = -2(445) = -890 \text{ cal/mol } O_2.$$

Then, $P = \exp(-\Delta G^\circ_T/RT) = \exp[890/(1.987 \times 500)] = 2.449 \approx 2.45$ atm.

An oxygen pressure in the system greater than 2.45 atm would prevent the decomposition from occurring.

Method 2

For tabulations that include values of Kf, the equilibrium constant for a formation reaction, the equilibrium constant for the desired reaction can also be determined from

$$Ka = \underset{\text{products}}{\prod Kf_i^{\nu_i}} \Big/ \underset{\text{reactants}}{\prod Kf_i^{\nu_i}}$$

where $\prod$ represents a continuous product. Thus, for the decomposition reaction being considered,

$$Ka = Kf^4_{Ag(c)} Kf_{O_2(g)} / Kf^2_{Ag_2O(c)},$$

or since Kf is by definition unity for any element,

$$Ka = Kf^{-2}_{Ag_2O(c)}.$$

From the tables, $\log_{10}Kf_{Ag_2O(c)} = -0.195;$

thus $Kf_{Ag_2O(c)} = 0.638$

and $Ka = (0.638)^{-2} \simeq 2.45.$

This is the same as the result of method 1.

Method 3

The standard-state change in the Gibbs energy for the desired reaction can also be determined from the tabulated values of $(G^\circ - H^\circ_{298})/T$ by noting that

$$\Delta G^\circ_T = T\Delta[(G^\circ - H^\circ_{298})/T] + \Delta H^\circ_{298},$$

where $$\Delta[(G^\circ - H^\circ_{298})/T] = \underset{\text{(products)}}{\Sigma\nu_i(G^\circ - H^\circ_{298})/T} - \underset{\text{(reactants)}}{\Sigma\nu_i(G^\circ - H^\circ_{298})/T}.$$

For the reaction of interest,

$$\Delta H^\circ_{298} = -2\Delta Hf^\circ_{Ag_2O(c)_{298}} = -2(-7420) \text{ cal},$$

$$\left.\begin{aligned}(G^\circ - H^\circ_{298})/T \text{ for } Ag_2O(c) &= -30.902 \text{ cal/mol},\\ (G^\circ - H^\circ_{298})/T \text{ for } Ag(c) &= -10.863 \text{ cal/mol},\\ \text{and } (G^\circ - H^\circ_{298})/T \text{ for } O_2(g) &= -49.813 \text{ cal/mol}.\end{aligned}\right\} \text{ at 500 K}$$

Then $\Delta G^\circ_{500} = 500[4(-10.863) + (-49.813) - 2(-30.902)] - 2(-7420)$

$= -890.5$ cal/mol $O_2(g)$.

This result differs from that in method 1 by only 0.5 cal, and this difference is again caused by round-off error in the tabulated values.

Method 4

The value of ΔG° for the reaction of interest can also be calculated from the equations for ΔGf° given in the tables. In this case

$$\Delta G^\circ_T = -2\Delta Gf^\circ_{Ag_2O(c),T}$$

and $$\Delta Gf^\circ_{Ag_2O(c)} = -7879 + 0.630\ T\ \ln T - 3.368\times10^{-3}T^2 + 51.80\times10^3/T + 14.214\ T,$$

where T is in K and ΔGf° is in cal/mol.

Thus $$\Delta G^\circ_T = 15758 - 1.260\ T\ \ln T + 6.736\times10^{-3}T^2 - 103.6\times10^3/T - 28.428\ T.$$

For 500 K, this equation gives

$$\Delta G^{\circ}_{500} = -894.4 \text{ cal/mol of } O_2(g).$$

Here again, note the small difference between this value and those calculated directly from the tabulated values. The difference is the result of using standard-form equations, rather than the more accurate equations used to calculate the tabulated values.

Method 5

As indicated in example 4, if this type of calculation were to be done by computer, or for many different temperatures, it would be more convenient to have an equation for ΔG°_T. The method of deriving the equation will be illustrated here. For the standard form of the heat capacity equation given in this bulletin,

$$Cp = a + bT + c/T^2,$$

the equations for ΔH°_T and ΔG°_T will have the form (145, p. 165)

$$\Delta H^{\circ}_T = \Delta H^{\circ}_o + \Delta a\ T + \Delta b\ T^2/2 - \Delta c/T$$

$$\text{and} \quad \Delta G^{\circ}_T = \Delta H^{\circ}_o - \Delta a\ T\ \ln T - \Delta b\ T^2/2 - \Delta c/2T + IT.$$

Here, as in example 4, method 3, Δa, Δb, and Δc are calculated from the heat capacity equations, that is,

$$\Delta a = \underset{\text{products}}{\Sigma \nu_i a_i} - \underset{\text{reactants}}{\Sigma \nu_i a_i}$$

and ΔH°_o and I are constants that must be determined. The constant ΔH°_o must be determined by inserting a known value of ΔH°_T at some temperature into the equation for the standard-state enthalpy change, as was illustrated in example 4. The constant I in the equation for the standard-state change in the Gibbs energy is determined in an analogous manner by using a known value of ΔG°_T at some temperature. These known values are frequently those of a temperature of 298 K, but they need not be. These calculations are illustrated below for the reaction being considered. The basic calculations are set up in tabular form. For this reaction,

$$\Delta a = 4\ a_{Ag(c)} + a_{O_2(g)} - 2\ a_{Ag_2O(c)}.$$

The expressions for Δb, Δc, ΔH°_{298}, and ΔG°_{298} are in a similar form, where ΔH°_{298} and ΔG°_{298} are calculated from the values for the formation equations.

	a	b x 10^3	c x 10^{-3}	ΔHf°_{298}	ΔGf°_{298}
Ag(c)	5.272	1.836	22.20	0	0
$O_2(g)$	7.230	1.006	-45.20	0	0
$Ag_2O(c)$	13.529	10.910	-81.80	-7420	-2697
Δ	+1.260	-13.470	+207.20	+14840	+5394

Then, $$\Delta H^{\circ}_T = \Delta H^{\circ}_o + 1.260\ T - 13.470 \times 10^{-3} T^2/2 - 207.20 \times 10^3/T.$$

The constant ΔH_o° can be evaluated by substituting the known value of ΔH_{298}° into the equation along with a value for T of 298.15 K:

$$14840 = \Delta H_o^\circ + 1.260(298.15) - 6.735\text{x}10^{-3}(298.15)^2 - 207.20\text{x}10^3/298.15.$$

Solving gives $\Delta H_o^\circ = 15758$ cal.

The expression for ΔG_T° can now be written as

$$\Delta G_T^\circ = 15758 - 1.260\ T\ \ln T + 6.735\text{x}10^{-3}T^2 - 207.20\text{x}10^3/2T + IT,$$

and the constant I can be determined by substituting the known value of ΔG_T° into the equation along with a value for T of 298.15 K,

$$5394 = 15758 - 1.260(298.15)\ \ln(298.15) + 6.735\text{x}10^{-3}(298.15)^2 - 103.60\text{x}10^3/298.15 + I(298.15).$$

This equation can be solved for I to give

$$I = -28.425 \text{ cal/K},$$

and the complete equation for ΔG_T° now becomes

$$\Delta G_T^\circ = 15758 - 1.260\ T\ \ln T + 6.735\text{x}10^{-3}T^2 - 103.60\text{x}10^3/T - 28.425\ T.$$

Note that this is the same equation as that used in method 4 above, within round-off error on the coefficients of the T and T^2 terms. The equation may be used to calculate a value of ΔG_T° for any temperature within the range of validity of the heat capacity equations. For a temperature of 500 K, this equation gives

$$\Delta G_{500}^\circ = -893.15 \text{ cal/mol } O_2(g).$$

Example 9

In example 5 the reaction of carbon with carbon dioxide at 1300 K was considered:

$$C(gr) + CO_2(g) = 2\ CO(g).$$

In the statement of the example, it was specified that the equilibrium conversion to carbon monoxide was very nearly 100 pct. This statement can now be proven.

For this reaction at 1300 K and 1 atm, where the ideal gas law is valid,

$$Ka = \overline{P}_{CO(g)}{}^2/[\overline{P}_{CO_2(g)}a_{C(gr)}] = \exp(-\Delta G_{1300}^\circ/RT).$$

For this pressure, $a_{C(gr)} = 1$, and the partial pressure can be evaluated, from its definition, as the product of the mole fraction, y_i, and the total pressure, P.

Thus, $$Ka = y_{CO(g)}^2 P/y_{CO_2(g)} = \exp(-\Delta G_{1300}^\circ/RT).$$

In this case $$\Delta G^\circ_{1300} = 2\Delta Gf^\circ_{CO(g)_{1300}} - \Delta Gf^\circ_{CO_2(g)_{1300}},$$

and from the tabulated values, this becomes

$$\Delta G^\circ_{1300} = 2(-54123) - (-94688) = -13558 \text{ cal/mol } CO_2(g),$$

so that $$Ka = \exp[13558/(1.987 \times 1300)] = 190.3.$$

Since the total pressure, P, is 1 atm, the two equations that must be solved simultaneously are

$$y^2_{CO(g)}/y_{CO_2(g)} = 190.3$$

and $$y_{CO(g)} + y_{CO_2(g)} = 1, \text{ by definition of } y_i.$$

Substitution of the second equation into the equilibrium expression to eliminate $y_{CO_2(g)}$ and solution of the resulting quadratic equation for $y_{CO(g)}$ will give

$$y_{CO(g)} \simeq 0.995$$

and $$y_{CO_2(g)} \simeq 0.00520.$$

The conversion of the original carbon dioxide can be calculated from the stoichiometry of the reaction. For 1 mol of gas at equilibrium, the feed consisted of (0.995/2 + 0.00520) mol of $CO_2(g)$, and (0.995/2) mol of $CO_2(g)$ was converted. Therefore, the conversion is

$$100[0.995/2]/[(0.995/2) + 0.00520] = 98.96 \text{ pct}.$$

The assumption made as a simplification in example 5 to ignore the 1 pct of the carbon dioxide that was not converted thus seems justified. Of course, one could now recalculate the values in example 5 for the actual equilibrium stoichiometry.

Example 10

In example 6 the reaction of carbon dioxide with carbon at 1300 K was considered:

$$C(gr) + CO_2(g) = 2\ CO(g).$$

However, the feed to the reactor was 80 pct $CO_2(g)$ and 20 pct $CO(g)$. Again, complete conversion to carbon monoxide was assumed. That assumption will be verified here.

In example 9, the following expression was developed for the reaction at 1300 K and 1 atm:

$$Ka = 190.3 = y^2_{CO(g)}/y_{CO_2(g)}.$$

Consider the case where 1 mol of gas is fed to the reactor; that is, 0.8 mol of $CO_2(g)$ and 0.2 mol of $CO(g)$. For a material balance, let x be the number of mols of $CO_2(g)$ that has reacted when the system reaches equilibrium. Then, the stoichiometry is conveniently done in tabular form.

Substance	Feed (mol)	Formed by reaction (mol)	Equilibrium (mol)
C(gr)	0.8	- x	0.8 - x
CO_2(g)	0.8	- x	0.8 - x
CO(g)	0.2	2x	0.2 + 2x
			(1 + x)gas

Thus, there is (1 + x) mole of gas in the system at equilibrium, and the mole fractions in the gas phase at equilibrium can be expressed as

$$y_{CO(g)} = (0.2 + 2x)/(1 + x)$$

and

$$y_{CO_2(g)} = (0.8 - x)/(1 + x).$$

Substitution of these values into the expression describing the equilibrium conditions gives

$$190.3 = (0.2 + 2x)^2/[(1 + x)(0.8 - x)].$$

This expression may be solved for x to give

$$x = 0.7907$$

and

$$y_{CO(g)} = (0.2 + 2x)/(1 + x) \approx 0.995$$

$$y_{CO_2(g)} = (0.8 - x)/(1 + x) \approx 0.0052.$$

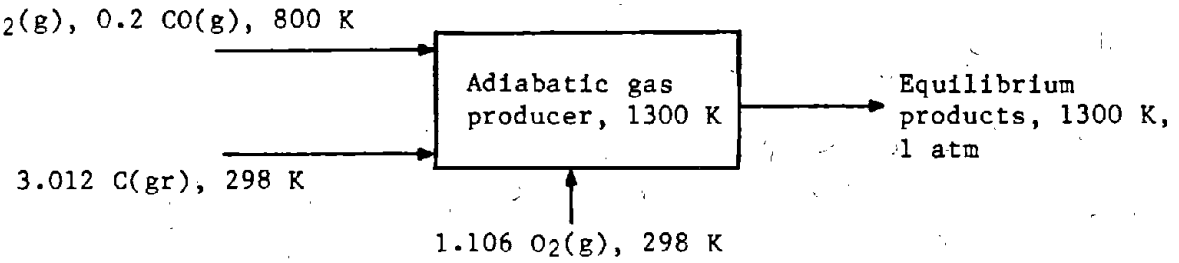
The conversion of carbon dioxide can be calculated as

$$\text{pct conversion} = (x/0.8)100 = 98.84 \text{ pct}.$$

Note that the assumption of complete conversion in example 6 is justified since it is very nearly true, and this assumption certainly simplifies the calculations. The equilibrium composition here is the same as that calculated in example 9. This must be true for this system because equilibrium composition is fixed at a given temperature and pressure, as shown by Gibbs' Phase Rule. The composition is fixed, but the conversion of carbon dioxide will change, depending upon the feed. This can be seen by comparing the results of examples 9 and 10.

Example 11

The results of example 7 represent the net process depicted below.



The amounts of oxygen and carbon fed were calculated by assuming that the following two reactions were complete:

$$CO_2(g) + C(gr) = 2\ CO(g)$$

$$0.5\ O_2(g) + C(gr) = CO(g).$$

Here again, the assumption of complete conversion at 1300 K and 1 atm will be checked.

The first reaction (rxn) was considered in example 9, and the results for 1300 K and 1 atm were

$$Ka_{(rxn\ 1)_{1300}} = 190.3 = y^2_{CO(g)}/y_{CO_2(g)}.$$

For the second reaction, since the ideal gas law will be valid,

$$Ka_{(rxn\ 2)} = \overline{P}_{CO(g)}/[\overline{P}_{O_2(g)}{}^{0.5}\ a_{C(gr)}].$$

For this pressure, $a_{C(gr)} \simeq 1$, and partial pressure can again be evaluated as the product of mole fraction, y_i, and total pressure, P. Thus, this expression becomes

$$Ka_{(rxn\ 2)} = [y_{CO(g)}/y_{O_2(g)}{}^{0.5}]P^{0.5}.$$

Note that P = 1 atm for this case.

The equilibrium constant is most easily evaluated by noting that the second reaction is just the formation reaction for CO(g). Thus,

$$Ka_{(rxn\ 2)_{1300}} = Kf_{CO(g)_{1300}}.$$

From the table for carbon monoxide

$$\log_{10}Kf_{Co(g)_{1300}} = 9.099.$$

Then $$Ka_{(rxn\ 2)_{1300}} = 1.256 \times 10^9.$$

At this point, we have two expressions representing reaction equilibria:

$$190.3 = y_{CO(g)}{}^2/y_{CO_2(g)}$$

and $$1.256 \times 10^9 = y_{CO(g)}/y_{O_2(g)}{}^{0.5}.$$

If it is also noted that

$$1 = y_{CO_2(g)} + y_{CO(g)} + y_{O_2(g)},$$

these equations can be solved simultaneously to give the equilibrium composition. The results are

$$y_{CO(g)} \simeq 0.995,$$

$$y_{CO_2(g)} \simeq 0.00520,$$

and $$y_{O_2(g)} \simeq 6.28 \times 10^{-19}.$$

The amount of oxygen present in the product is extremely small. If this figure is taken as zero, and the results for CO(g) and CO_2(g) are compared with the results of example 10, it can be seen that the conversion of CO_2(g) will again be close to 99 pct. One should note, however, that these calculations have been done in a particular manner: In example 7, complete conversion was assumed, and in this example, this assumption was simply checked and found to be valid. This approach is workable only because the assumption made in example 7 was valid.

Suppose, however, that the conversion in the first reaction (or possibly both reactions) was not nearly 100 pct. The proper method of calculation would then require the consideration of three expressions and the energy balance for the adiabatic reactor. Algebraic unknowns could be defined in a manner similar to that illustrated in example 10, and these algebraic unknowns could be related to the mole fraction by stoichiometric methods. The resulting equations could then be solved for the algebraic unknowns, and thus for the appropriate conversions and equilibrium mole fractions. This technique is too cumbersome for illustration here, but it should be used for accurate solution to complex cases where the assumption of complete conversion is not valid.

Example 12

Many substances exist in more than one form in the vapor phase. The vapor composition can be calculated, as can the vapor pressure for mixed-species systems. This will be illustrated for the simple vaporization of bismuth at 900 K to form both Bi(g) and Bi_2(g). The reactions of interest are

$$Bi(l) = Bi(g)$$

and $$2\ Bi(l) = Bi_2(g).$$

For a temperature of 900 K and the relatively low pressure expected, the gas phase can be treated as an ideal gas. As a result, the activities of the gaseous species can again be evaluated as partial pressures. In addition, for the low pressure expected, the activity of pure liquid bismuth can be approximated as $a_{Bi(l)} \simeq 1$. The equilibrium expressions for these two reactions then become

$$Ka_{(rxn\ 1)} = \overline{P}_{Bi(g)} = y_{Bi(g)}P$$

and $$Ka_{(rxn\ 2)} = \overline{P}_{Bi_2(g)} = y_{Bi_2(g)}P.$$

These constants are most easily evaluated by noting that the first reaction is the formation reaction for Bi(g), and the second reaction is the formation reaction for Bi_2(g). Thus,

$$Ka_{(rxn\ 1)_{900}} = Kf_{Bi(g)_{900}}$$

and $$Ka_{(rxn\ 2)_{900}} = Kf_{Bi_2(g)_{900}}.$$

From the tables for Bi(g) and Bi_2(g),

$$\log_{10} Kf_{Bi(g)_{900}} = -5.798$$

and $$\log_{10} Kf_{Bi_2(g)_{900}} = -5.661.$$

Then $$Ka_{(rxn\ 1)_{900}} = 1.592 \times 10^{-6}$$

and $$Ka_{(rxn\ 2)_{900}} = 2.183 \times 10^{-6}.$$

At this point, we have two expressions representing the reaction equilibria:

$$y_{Bi(g)} P = 1.592 \times 10^{-6}$$

and $$y_{Bi_2(g)} P = 2.183 \times 10^{-6}.$$

It is also noted that

$$y_{Bi(g)} + y_{Bi_2(g)} = 1.$$

These expressions can be solved simultaneously to give the equilibrium composition of the gas phase and the total pressure above the liquid bismuth; i.e., the vapor pressure. The results are

$$y_{Bi(g)} = 0.422,$$

$$y_{Bi_2(g)} = 0.578,$$

and $$P = 3.775 \times 10^{-6} \text{ atm}.$$

For this low pressure, the assumptions of ideal-gas behavior and unit activity of the pure liquid are valid. A significant error would obviously be incurred if one ignored the fact that there is more than one gaseous species. In this case, for example, if one assumed that the gas was only Bi(g) and considered only the first reaction with $y_{Bi(g)} = 1$, the calculated vapor pressure would be 1.592×10^{-6} atm, an error of 57.8 pct.

Example 13

The standard-state change in the Gibbs energy for a reaction can be related to the equilibrium potential for an electrolytic cell in which the reaction occurs by

$$\Delta G^\circ = - nFe^\circ,$$

where e° is the equilibrium potential in volts, n is the number of equivalents involved in the overall reaction, ΔG° is the standard state change in the Gibbs energy in calories, and F is Faraday's constant (23060.9 cal/volt-equivalent).

Consider the cell Pt, Cu, Cu_2O || ZrO_2 || O_2(1 atm),

for which the overall reaction is

$$2\ Cu(c) + 0.5\ O_2(g) = Cu_2O(c).$$

Determine the equilibrium potential at 1000 K.

For the overall reaction involved,

$$\Delta G^\circ_{1000} = \Delta Gf^\circ_{Cu_2O(c)_{1000}} = -22867 \text{ cal/mol},$$

from the tabulated data for $Cu_2O(c)$. In addition, n = 2.

Thus, $$e^\circ = -\Delta G^\circ/nF = 22866/[2(23060.9)] = 0.496 \text{ volt}.$$

This is the equilibrium potential that would be measured for the given cell. Indeed, the measurement of this potential, whether by direct or indirect methods, is one very useful method of determining ΔG°.

Example 14

The significance of the change in the standard-state Gibbs energy for a reaction can be seen by returning to the reactions considered in previous examples. In addition, the limitations on the conclusions that can be made solely on the basis of equilibrium considerations can be noted.

In example 8, the decomposition of silver oxide was considered:

$$2\ Ag_2O(c) = 4\ Ag(c) + O_2(g).$$

It was shown that, for relatively low pressure, the equilibrium constant was numerically equal to the partial pressure of oxygen at equilibrium, in atmospheres; i.e.,

$$Ka = \overline{P}_{O_2}.$$

The methods illustrated in example 8 allow the calculation of the change in the standard-state Gibbs energy and the equilibrium constant for this reaction for any desired temperature. Several such values are given below:

T, K	ΔG°(cal)	$\overline{P}_{O_2}$(atm)
350	+3758	0.0045
400	+2190	.064
450	+ 638	.490
500	- 890	2.45

It is obvious from these results that as ΔG° becomes more negative, i.e., algebraically smaller, the equilibrium constant becomes larger. This is simply the direct consequence of the relationship between Ka and ΔG° as given in equation 7. However, these results alone are not sufficient to indicate whether the reaction will occur, and, if so, to what extent. In this case, the reaction will not occur at all if a partial pressure of oxygen is maintained in the system that is larger than the equilibrium value; e.g., greater than 2.45 atm at 500 K, or greater than 0.064 atm at 400 K. Thus, silver oxide would not decompose in air at 400 K. Conversely, the reaction could proceed if the partial pressure of oxygen in the system is maintained at a value less than the equilibrium value. Silver oxide could decompose in air at 500 K; decomposition could also occur at 400 K if the system were swept with an inert gas such as argon so that the oxygen pressure was below 0.064 atm.

In examples 9 and 10, the calculation of equilibrium conversion for the following reaction was illustrated:

$$C(gr) + CO_2(g) = 2\ CO(g).$$

The equilibrium constant was shown to have the form

$$Ka = y^2_{CO(g)}\ P/y_{CO_2(g)}.$$

For a temperature of 1000 K,

$$\Delta G^\circ_{1000} = -1095 \text{ cal}$$

and

$$Ka = 1.735.$$

The methods illustrated in examples 9 and 10 allow the calculation of equilibrium conversion as a function of pressure for this temperature. The results for several pressures are given below for a feed consisting of stoichiometric amounts of carbon and carbon dioxide.

P(atm)	Equilibrium conversion, pct
1	30.3
2	17.8
5	8.0
10	4.2

It should be noted that the value of the equilibrium constant, Ka, is independent of pressure. It is the same for all four sets of conditions above. However, the equilibrium conversion, and thus the composition, is very strongly dependent upon pressure for this reaction.

These two short calculations lead indirectly to the consideration of the "feasibility" of a chemical reaction. The only information one can derive from the standard-state change in the Gibbs energy for a reaction is really the magnitude of the equilibrium constant. Certainly this is an important consideration, for the attainment of equilibrium is the limitation on the extent to which a reaction can proceed. However, the value of ΔG° or Ka is not a sufficient basis for reaching a conclusion. As seen above, the equilibrium conversion is affected by the presence of an inert gas in some cases, or by pressure in others. A comparison of the results of examples 9 and 10 will also show the effect of feed composition.

Equilibrium conditions represent the best case; i.e., the maximum extent to which a reaction will proceed. The kinetics of the reaction is the second controlling factor that must be considered. Neither equilibrium considerations nor kinetics is sufficient by itself. Neither very slow reactions with large equilibrium constants nor very fast reactions with very small equilibrium constants are really "feasible."

It is important to consider both thermodynamics and kinetics when attempting to assess commercial feasibility. Care should be used if the magnitude and sign of the standard-state change in the Gibbs energy is used as a guide.

THERMODYNAMIC DATA FOR ELEMENTS AND OXIDES

In this section, thermodynamic values for the elements and oxides are given in both tabular and equation forms. The tables have the base temperature, 298.15 K, and are not extended much above the temperature of the available data. Other than in tables or equations, the base temperature is usually abbreviated as 298 K. To avoid confusion, the standard state at this base temperature is indicated in each table heading and in the chemical formation equation given for the oxides. The symbols c, l, g, and vit refer respectively to crystal, liquid, gas, and vitreous phases. Also, the Greek letters α, β, γ, δ, and ε are used to denote different crystalline forms. In a few instances, Greek letters also denote substances above and below a second order transformation. Again, to avoid confusion, where substances have the same chemical formula but have different standard states, the standard state is explicity given in the heading. Some examples are:

Eu_2O_3(cubic) - Eu_2O_3(monoclinic), TiO_2(rutile) - TiO_2(anatase), and P(white) - P(red).

Many of the experimental measurements of thermodynamic properties used in this compilation were obtained using the International Practical Temperature Scale of 1948 (IPTS - 48). This scale has been superseded by IPTS - 68 (38) and the amended edition of 1975 (39). These scales differ by as much as 2.6 K (at 2000 K), but no attempt has been made, except as specifically noted, to convert earlier measurements to IPTS - 68 since the errors involved are less than experimental errors.

The tables are arranged in alphabetical order by chemical symbols. For convenience, the chemical symbol of the pertinent element has been included in pagination.

Ag(c,1)

Silver

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.070	10.170	10.170	0
300	6.072	10.208	10.171	.011
400	6.170	11.965	10.408	.623
500	6.297	13.355	10.863	1.246
600	6.436	14.515	11.380	1.881
700	6.587	15.518	11.901	2.532
800	6.751	16.409	12.409	3.200
900	6.927	17.214	12.897	3.885
1000	7.116	17.953	13.367	4.586
1100	7.316	18.641	13.816	5.307
1200	7.530	19.286	14.245	6.049
1235.08	7.607	19.508	14.395	6.315
1235.08	8.000	21.694	14.395	9.015
1300	8.000	22.104	14.770	9.534
1400	8.000	22.697	15.316	10.334
1500	8.000	23.249	15.826	11.134
1600	8.000	23.765	16.306	11.934
1700*	8.000	24.250	16.759	12.734
1800	8.000	24.707	17.188	13.534
1900	8.000	25.140	17.596	14.334
2000	8.000	25.550	17.983	15.134

*Data above 1600 K extrapolated.

Phase changes: 1235.08 K, melting point of Ag; ΔH° = 2.700 kcal/mol.
2440 K, boiling point of Ag; ΔH° = 59.9 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1235.08 K: $Cp^\circ = 5.272 + 1.836\times10^{-3}T + 0.222\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.272\times10^{-3}T + 0.918\times10^{-6}T^2 - 0.222\times10^{2}T^{-1} - 1.579$

1235.08-2000 K: $Cp^\circ = 8.000$

$H^\circ - H^\circ_{298} = 8.000\times10^{-3}T - 0.866$

Sources: Low-temperature heat capacities and entropy at 298 K from Furukawa (73). All other data from Hultgren (99) who extrapolated above 1600 K by assuming constant heat capacity. Data corrected to IPTS-68.

Ag(g)

Silver (ideal monatomic gas)

[Formation: Ag(c,1) = Ag(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^{\circ}_{298})/T$	$H°-H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	4.968	41.321	41.321	0	68.090	58.802	-43.103
300	4.968	41.351	41.321	.009	68.088	58.745	-42.795
400	4.968	42.781	41.516	.506	67.973	55.647	-30.403
500	4.968	43.889	41.883	1.003	67.847	52.580	-22.982
600	4.968	44.795	42.295	1.500	67.709	49.541	-18.045
700	4.968	45.561	42.710	1.996	67.554	46.524	-14.525
800	4.968	46.224	43.108	2.493	67.383	43.531	-11.892
900	4.968	46.809	43.487	2.990	67.195	40.559	-9.849
1000	4.968	47.333	43.846	3.487	66.991	37.611	-8.220
1100	4.968	47.806	44.184	3.984	66.767	34.685	-6.891
1200	4.968	48.239	44.506	4.480	66.521	31.777	-5.787
1235.08	4.968	48.382	44.614	4.654	66.429	30.767	-5.444
1235.08	4.968	48.382	44.614	4.654	63.729	30.767	-5.444
1300	4.968	48.636	44.808	4.977	63.533	29.041	-4.882
1400	4.968	49.004	45.094	5.474	63.230	26.400	-4.121
1500	4.968	49.347	45.366	5.971	62.927	23.780	-3.465
1600	4.968	49.668	45.625	6.468	62.624	21.179	-2.893
1700	4.968	49.969	45.873	6.964	62.320	18.598	-2.391
1800	4.968	50.253	46.108	7.461	62.017	16.034	-1.947
1900	4.968	50.522	46.334	7.958	61.714	13.488	-1.551
2000	4.968	50.776	46.549	8.455	61.411	10.959	-1.198

Phase change: 1235.08 K, melting point of Ag; $\Delta H° = 2.700$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.968$

$H°-H^{\circ}_{298} = 4.968\times10^{-3}T - 1.481$

Formation equations (kcal/mol):

298.15-1235.08 K: $\Delta Hf° = 68.188 - 0.304\times10^{-3}T - 0.918\times10^{-6}T^2 + 22.200T^{-1}$

$\Delta Gf° = 68.188 + 0.304\times10^{-3}T\ln T + 0.918\times10^{-6}T^2 + 11.100T^{-1} - 33.610\times10^{-3}T$

1235.08-2000 K: $\Delta Hf° = 67.475 - 3.032\times10^{-3}T$

$\Delta Gf° = 67.475 + 3.032\times10^{-3}T\ln T - 51.312\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (36). All other data from Hilsenrath (94).

$Ag_2O(c)$

Disilver Oxide

[Formation: $2Ag(c) + 0.5O_2(g) = Ag_2O(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	15.862	29.000	29.000	0	-7.420	-2.697	1.977
300	15.893	29.098	29.001	.029	-7.420	-2.667	1.943
350	16.683	31.609	29.198	.844	-7.390	-1.879	1.173
400	17.386	33.883	29.643	1.696	-7.332	-1.095	.598
450	18.031	35.969	30.231	2.582	-7.246	-.319	.155
500*	18.637	37.900	30.902	3.499	-7.140	.445	-.195

*Ag_2O decomposes near 500 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-500 K: $Cp° = 13.529 + 10.910\times10^{-3}T - 0.818\times10^{5}T^{-2}$

$H°- H°_{298} = 13.529\times10^{-3}T + 5.455\times10^{-6}T^{2} + 0.818\times10^{2}T^{-1} - 4.793$

Formation equations (kcal/mol):

298.15-500 K: $\Delta Hf° = -7.879 - 0.630\times10^{-3}T + 3.368\times10^{-6}T^{2} + 103.600T^{-1}$

$\Delta Gf° = -7.879 + 0.630\times10^{-3}T\ln T - 3.368\times10^{-6}T^{2} + 51.800T^{-1} + 14.214\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). Low-tempature heat capacity and entropy at 298 K based on Gerkin (75) and Gregor (82). High-temperature data based on Kobayashi (137).

$Ag_2O_2(c)$

Disilver Dioxide, Silver Peroxide

[Formation: $2Ag(c) + O_2(g) = Ag_2O_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	21.000	28.000	28.000	0	-5.800	6.527	-4.784
300*	21.040	28.130	28.000	.039	-5.796	6.605	-4.811
400	22.710	34.460	28.860	2.240	-5.529	10.695	-5.843
500	23.640	39.630	30.510	4.560	-5.186	14.714	-6.432

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-500 K: $Cp° = 17.819 + 11.958\times10^{-3}T$

$H°- H°_{298} = 17.819\times10^{-3} + 5.979\times10^{-6}T^2 - 5.844$

Formation equations (kcal/mol):

298.15-500 K: $\Delta Hf° = -6.134 + 0.045\times10^{-3}T + 3.640\times10^{-6}T^2 - 0.800T^{-1}$

$\Delta Gf° = -6.134 - 0.045\times10^{-3}T\ln T - 3.640\times10^{-6}T^2 - 0.400T^{-1} + 43.812\times10^{-3}T$

Sources: Enthalpy of formation, heat capacity, and entropy at 298 K from Wagman (237). High temperature data estimated.

Al(c,1)

Aluminum

T, K	cal/mol•K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.820	6.776	6.776	0
300	5.830	6.812	6.776	.011
400	6.120	8.530	7.007	.609
500	6.380	9.922	7.456	1.233
600	6.660	11.110	7.970	1.884
700	7.000	12.161	8.495	2.566
800	7.390	13.120	9.014	3.285
900	7.770	14.014	9.520	4.045
933.61	8.060	14.303	9.687	4.310
933.61	7.590	17.067	9.687	6.890
1000	7.590	17.589	10.194	7.395
1100	7.590	18.312	10.899	8.154
1200	7.590	18.973	11.545	8.913
1300	7.590	19.580	12.140	9.672
1400	7.590	20.143	12.692	10.431
1500	7.590	20.666	13.206	11.190
1600	7.590	21.156	13.688	11.949
1700	7.590	21.616	14.141	12.708
1800	7.590	22.050	14.568	13.467
1900*	7.590	22.461	14.974	14.226
2000	7.590	22.850	15.358	14.985
2100	7.590	23.220	15.723	15.744
2200	7.590	23.573	16.072	16.503
2300	7.590	23.911	16.406	17.262
2400	7.590	24.234	16.725	18.021
2500	7.590	24.544	17.032	18.780

*Data above 1800 K extrapolated.

Phase changes: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
2798 K, boiling point of Al; ΔH° = 70.1 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-933.61 K: $Cp^\circ = 4.592 + 3.454\times10^{-3}T + 0.174\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.592\times10^{-3}T + 1.727\times10^{-6}T^2 - 0.174\times10^{2}T^{-1} - 1.464$

933.61-2500 K: $Cp^\circ = 7.590$

$H^\circ - H^\circ_{298} = 7.590\times10^{-3}T - 0.196$

Sources: Entropy at 298 K from CODATA (36). Other data from Hultgren (99) who extrapolated above 1800 K by assuming constant heat capacity. Data corrected to IPTS-68.

Al(g)

Aluminum (ideal monatomic gas)

[Formation: Al(c,l) = Al(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.112	39.302	39.302	0	78.800	69.102	-50.653
300	5.111	39.335	39.305	.009	78.798	69.041	-50.296
400	5.047	40.794	39.501	.517	78.708	65.802	-35.952
500	5.018	41.917	39.877	1.020	78.587	62.589	-27.357
600	5.002	42.830	40.295	1.521	78.437	59.405	-21.638
700	4.993	43.600	40.713	2.021	78.255	56.248	-17.561
800	4.987	44.266	41.116	2.520	78.035	53.118	-14.511
900	4.983	44.854	41.501	3.018	77.773	50.017	-12.146
933.61	4.982	45.037	41.625	3.185	77.675	48.982	-11.466
933.61	4.982	45.037	41.625	3.185	75.095	48.982	-11.466
1000	4.980	45.378	41.862	3.516	74.921	47.132	-10.301
1100	4.978	45.853	42.204	4.014	74.660	44.365	-8.814
1200	4.976	46.286	42.526	4.512	74.399	41.623	-7.581
1300	4.975	46.684	42.831	5.009	74.137	38.902	-6.540
1400	4.974	47.053	43.119	5.507	73.876	36.202	-5.651
1500	4.973	47.396	43.393	6.004	73.614	33.519	-4.884
1600	4.972	47.717	43.654	6.501	73.352	30.854	-4.214
1700	4.972	48.018	43.901	6.999	73.091	28.208	-3.626
1800	4.972	48.302	44.138	7.496	72.829	25.575	-3.105
1900	4.971	48.571	44.364	7.993	72.567	22.958	-2.641
2000	4.971	48.826	44.581	8.490	72.305	20.353	-2.224

Phase change: 933.61 K, melting point of Al; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.966 + 0.131\times10^{5}T^{-2}$

$H°- H°_{298} = 4.966\times10^{-3}T - 0.131\times10^{2}T^{-1} - 1.437$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = 78.828 + 0.374\times10^{-3}T - 1.727\times10^{-6}T^{2} + 4.300T^{-1}$

$\Delta Gf° = 78.828 - 0.374\times10^{-3}T\ln T + 1.727\times10^{-6}T^{2} + 2.150T^{-1} - 31.027\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = 77.560 - 2.624\times10^{-3}T - 13.100T^{-1}$

$\Delta Gf° = 77.560 + 2.624\times10^{-3}T\ln T - 6.550T^{-1} - 48.550\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (36). All other data from Hultgren (99).

AlO(g)

Aluminum Monoxide (ideal gas)

[Formation: $Al(c,l) + 0.5O_2(g) = AlO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.381	52.169	52.169	0	16.400	10.171	-7.456
300	7.388	52.214	52.169	.014	16.396	10.133	-7.382
400	7.765	54.392	52.462	.772	16.201	8.075	-4.412
500	8.066	56.159	53.031	1.564	16.004	6.066	-2.651
600	8.290	57.651	53.681	2.382	15.793	4.098	-1.493
700	8.460	58.942	54.342	3.220	15.560	2.167	-.677
800	8.604	60.081	54.989	4.074	15.296	.272	-.074
900	8.743	61.102	55.612	4.941	14.997	-1.589	.386
933.61	8.793	61.423	55.815	5.236	14.888	-2.206	.516
933.61	8.793	61.423	55.815	5.236	12.308	-2.206	.516
1000	8.892	62.031	56.208	5.823	12.115	-3.232	.706
1100	9.057	62.886	56.777	6.720	11.833	-4.753	.944
1200	9.241	63.682	57.319	7.635	11.565	-6.248	1.138
1300	9.440	64.430	57.839	8.568	11.312	-7.725	1.299
1400	9.650	65.137	58.335	9.523	11.076	-9.179	1.433
1500	9.863	65.810	58.811	10.499	10.858	-10.619	1.547
1600	10.073	66.453	59.269	11.495	10.656	-12.044	1.645
1700	10.275	67.070	59.709	12.513	10.474	-13.457	1.730
1800	10.463	67.663	60.135	13.550	10.308	-14.860	1.804
1900	10.633	68.233	60.546	14.605	10.157	-16.252	1.869
2000	10.783	68.782	60.944	15.676	10.020	-17.638	1.927

Phase change: 933.61 K, melting point of Al; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.364 + 1.656\times10^{-3}T - 0.424\times10^{5}T^{-2}$

$H°- H°_{298} = 7.364\times10^{-3}T + 0.828\times10^{-6}T^{2} + 0.424\times10^{2}T^{-1} - 2.411$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = 16.629 - 0.843\times10^{-3}T - 1.150\times10^{-6}T^{2} + 37.200T^{-1}$

$\Delta Gf° = 16.629 + 0.843\times10^{-3}T\ln T + 1.150\times10^{-6}T^{2} + 18.600T^{-1} - 27.013\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = 15.361 - 3.841\times10^{-3}T + 0.577\times10^{-6}T^{2} + 19.800T^{-1}$

$\Delta Gf° = 15.361 + 3.841\times10^{-3}T\ln T - 0.577\times10^{-6}T^{2} + 9.900T^{-1} - 44.537\times10^{-3}T$

Source: Data from Chase (32).

$(AlO)_2(g)$

Dimeric Aluminum Monoxide (ideal gas)

[Formation: $2Al(c,l) + O_2(g) = (AlO)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.250	66.043	66.043	0	-104.000	-105.039	76.995
300	15.286	66.138	66.045	.028	-104.007	-105.047	76.525
400	16.786	70.759	66.664	1.638	-104.303	-105.347	57.558
500	17.699	74.610	67.878	3.366	-104.554	-105.576	46.147
600	18.276	77.892	69.280	5.167	-104.810	-105.755	38.521
700	18.657	80.740	70.719	7.015	-105.104	-105.889	33.060
800	18.919	83.249	72.132	8.894	-105.461	-105.980	28.952
900	19.107	85.489	73.493	10.796	-105.893	-106.021	25.745
933.61	19.153	86.190	73.938	11.439	-106.057	-106.023	24.819
933.61	19.153	86.190	73.938	11.439	-111.217	-106.023	24.819
1000	19.244	87.510	74.796	12.714	-111.502	-105.644	23.088
1100	19.349	89.349	76.036	14.644	-111.929	-105.037	20.869
1200	19.429	91.036	77.217	16.583	-112.356	-104.390	19.012
1300	19.493	92.594	78.341	18.529	-112.784	-103.711	17.435
1400	19.543	94.040	79.411	20.481	-113.214	-102.995	16.078
1500	19.585	95.390	80.432	22.437	-113.646	-102.254	14.898
1600	19.619	96.655	81.406	24.398	-114.080	-101.478	13.861
1700	19.647	97.845	82.339	26.361	-114.517	-100.677	12.943
1800	19.671	98.969	83.232	28.327	-114.957	-99.850	12.123
1900	19.691	100.033	84.088	30.295	-115.401	-98.996	11.387
2000	19.709	101.044	84.911	32.265	-115.848	-98.124	10.722

*Data except enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.651 + 0.774\times10^{-3}T - 3.228\times10^{5}T^{-2}$

$H°- H°_{298} = 18.651T + 0.387\times10^{-6}T^2 + 3.228\times10^{2}T^{-1} - 6.678$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -105.397 + 2.237\times10^{-3}T - 3.570\times10^{-6}T^2 + 312.400T^{-1}$

$\Delta Gf° = -105.397 - 2.237\times10^{-3}T\ln T + 3.570\times10^{-6}T^2 + 156.20T^{-1} + 11.125\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = -107.933 - 3.759\times10^{-3}T - 0.116\times10^{-6}T^2 + 277.600T^{-1}$

$\Delta Gf° = -107.933 + 3.759\times10^{-3}T\ln T + 0.116\times10^{-6}T^2 + 138.80T^{-1} - 23.922\times10^{-3}T$

Source: Data from Chase (32); who estimated all except enthalpy of formation at 298 K.

$AlO_2(g)$

Aluminum Dioxide (ideal gas)

[Formation: $Al(c,l) + O_2(g) = AlO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.684	58.608	58.608	0	-44.900	-45.743	33.530
300	11.707	58.680	58.608	.022	-44.902	-45.748	33.327
400	12.701	62.195	59.080	1.246	-44.986	-46.016	25.142
500	13.332	65.102	60.002	2.550	-45.037	-46.267	20.223
600	13.740	67.571	61.063	3.905	-45.088	-46.506	16.940
700	14.014	69.711	62.150	5.293	-45.160	-46.738	14.592
800	14.204	71.596	63.215	6.705	-45.265	-46.958	12.828
900	14.340	73.277	64.241	8.132	-45.412	-47.162	11.452
933.61	14.374	73.803	64.576	8.615	-45.471	-47.226	11.055
933.61	14.374	73.803	64.576	8.615	-48.051	-47.225	11.055
1000	14.441	74.793	65.221	9.572	-48.149	-47.163	10.307
1100	14.517	76.173	66.155	11.020	-48.299	-47.057	9.349
1200	14.576	77.439	67.044	12.474	-48.452	-46.938	8.548
1300	14.623	78.608	67.890	13.934	-48.607	-46.807	7.869
1400	14.661	79.693	68.694	15.399	-48.765	-46.661	7.284
1500	14.691	80.705	69.461	16.866	-48.927	-46.506	6.776
1600	14.717	81.654	70.193	18.337	-49.092	-46.338	6.329
1700	14.738	82.547	70.894	19.810	-49.260	-46.161	5.934
1800	14.757	83.390	71.566	21.284	-49.433	-45.973	5.582
1900	14.773	84.188	72.209	22.761	-49.609	-45.775	5.265
2000	14.788	84.947	72.827	24.239	-49.789	-45.571	4.980

*Data except enthalpy of formation at 298 K are estimated.

Phase change: 933.61 K, melting point of Al; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.004 + 0.552\times10^{-3}T - 2.208\times10^{5}T^{-2}$

$H°- H°_{298} = 14.004\times10^{-3}T + 0.276\times10^{-6}T^2 + 2.208\times10^{2}T^{-1} - 4.940$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -46.024 + 2.182\times10^{-3}T - 1.954\times10^{-6}T^2 + 193.000T^{-1}$

$\Delta Gf° = -46.024 - 2.182\times10^{-3}T\ln T + 1.954\times10^{-6}T^2 + 96.500T^{-1} + 11.708\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = -47.292 - 0.816\times10^{-3}T - 0.227\times10^{-6}T^2 + 175.600T^{-1}$

$\Delta Gf° = -47.292 + 0.816\times10^{-3}T\ln T + 0.227\times10^{-6}T^2 + 87.800T^{-1} - 5.816\times10^{-3}T$

Source: Data from Chase (32); who estimated all except enthalpy of formation at 298 K.

$Al_2O(g)$

Dialuminum Oxide (ideal gas)

[Formation: $2Al(c,l) + 0.5O_2(g) = Al_2O(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.513	61.414	61.414	0	-31.200	-38.165	27.975
300	12.528	61.491	61.414	.023	-31.205	-38.208	27.834
400	13.190	65.192	61.915	1.311	-31.469	-40.503	22.130
500	13.643	68.187	62.879	2.654	-31.739	-42.730	18.677
600	13.952	70.704	63.979	4.035	-32.038	-44.899	16.354
700	14.166	72.871	65.098	5.441	-32.385	-47.015	14.679
800	14.318	74.773	66.191	6.866	-32.797	-49.079	13.408
900	14.429	76.466	67.239	8.304	-33.286	-51.086	12.405
933.61	14.457	76.996	67.581	8.789	-33.468	-51.747	12.113
933.61	14.457	76.996	67.581	8.789	-38.628	-51.747	12.113
1000	14.512	77.991	68.240	9.751	-38.952	-52.670	11.511
1100	14.575	79.377	69.191	11.205	-39.436	-54.019	10.733
1200	14.625	80.648	70.093	12.666	-39.917	-55.322	10.075
1300	14.664	81.820	70.951	14.130	-40.399	-56.588	9.513
1400	14.696	82.908	71.767	15.598	-40.881	-57.814	9.025
1500	14.722	83.923	72.544	17.069	-41.362	-59.009	8.598
1600	14.743	84.874	73.285	18.542	-41.846	-60.170	8.219
1700	14.761	85.768	73.993	20.017	-42.330	-61.300	7.881
1800	14.776	86.612	74.671	21.494	-42.815	-62.401	7.576
1900	14.789	87.411	75.320	22.973	-43.301	-63.472	7.301
2000	14.800	88.170	75.944	24.452	-43.790	-64.523	7.051

Phase change: 933.61 K, melting point of Al; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.043 + 0.522\times10^{-3}T - 1.499\times10^{5}T^{-2}$

$H°- H°_{298} = 14.043\times10^{-3}T + 0.261\times10^{-6}T^2 + 1.499\times10^{2}T^{-1} - 4.713$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -31.808 + 1.244\times10^{-3}T - 3.445\times10^{-6}T^2 + 162.100T^{-1}$

$\Delta Gf° = -31.808 - 1.244\times10^{-3}T\ln T + 3.445\times10^{-6}T^2 + 81.050T^{-1} - 16.170\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = -34.344 - 4.752\times10^{-3}T + 0.010\times10^{-6}T^2 + 127.300T^{-1}$

$\Delta Gf° = -34.344 + 4.752\times10^{-3}T\ln T - 0.010\times10^{-6}T^2 + 63.650T^{-1} - 51.217\times10^{-3}T$

Source: Data from Chase (32).

$Al_2O_3(\alpha,1)$

Dialuminum Trioxide, α-Alumina

[Formation: $2Al(c,1) + 1.5O_2(g) = Al_2O_3(\alpha,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.885	12.170	12.170	0	-400.500	-378.172	277.204
300	18.981	12.287	12.170	.035	-400.507	-378.033	275.394
400	22.965	18.343	12.968	2.150	-400.652	-370.512	202.436
500	25.366	23.747	14.595	4.576	-400.571	-362.982	158.657
600	26.899	28.517	16.527	7.194	-400.388	-355.478	129.481
700	27.946	32.747	18.547	9.940	-400.172	-348.009	108.652
800	28.713	36.531	20.563	12.774	-399.974	-340.574	93.039
900	29.317	39.949	22.531	15.676	-399.813	-333.161	80.901
933.61	29.486	41.027	23.178	16.664	-399.769	-330.673	77.407
933.61	29.486	41.027	23.178	16.664	-404.929	-330.673	77.407
1000	29.821	43.065	24.431	18.634	-404.795	-325.397	71.115
1100	30.260	45.928	26.257	21.638	-404.568	-317.468	63.074
1200	30.653	48.578	28.008	24.684	-404.312	-309.560	56.378
1300	31.008	51.046	29.686	27.768	-404.030	-301.676	50.716
1400	31.329	53.356	31.295	30.885	-403.727	-293.813	45.866
1500	31.618	55.527	32.838	34.033	-403.402	-285.975	41.666
1600	31.874	57.576	34.321	37.208	-403.060	-278.157	37.994
1700	32.100	59.515	35.746	40.407	-402.702	-270.360	34.757
1800	32.297	61.356	37.119	43.627	-402.332	-262.585	31.882
1900	32.469	63.107	38.441	46.865	-401.953	-254.831	29.312
2000	32.623	64.776	39.716	50.120	-401.565	-247.099	27.001
2100	32.769	66.371	40.948	53.389	-401.171	-239.385	24.913
2200	32.918	67.899	42.138	56.674	-400.769	-231.691	23.016
2300	33.085	69.366	43.290	59.974	-400.361	-224.013	21.286
2327	33.135	69.752	43.594	60.870	-400.247	-221.941	20.844
2327	46.000	81.217	43.593	87.550	-373.567	-221.941	20.844
2400	46.000	82.638	44.760	90.908	-372.327	-217.202	19.779
2500	46.000	84.516	46.313	95.508	-370.634	-210.773	18.426

Phase changes: 933.61 K, melting point of Al; $\Delta H° = 2.580$ kcal/mol.
2327 K, melting point of Al_2O_3; $\Delta H° = 26.68$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2327 K: $Cp° = 27.605 + 2.758\times10^{-3}T - 8.482\times10^{5}T^{-2}$

$H°- H°_{298} = 27.605\times10^{-3}T + 1.379\times10^{-6}T^{2} + 8.482\times10^{2}T^{-1} - 11.198$

2327-2500 K: $Cp° = 46.000$

$H°- H°_{298} = 46.000\times10^{-3}T - 19.492$

$Al_2O_3(\alpha,l)$ - Continued

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = -405.241 + 7.576\times10^{-3}T - 2.830\times10^{-6}T^2 + 815.200T^{-1}$

$\Delta Gf^\circ = -405.241 - 7.576\times10^{-3}T\ln T + 2.830\times10^{-6}T^2 + 407.600T^{-1} + 128.529\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -407.777 + 1.580\times10^{-3}T + 0.624\times10^{-6}T^2 + 780.400T^{-1}$

$\Delta Gf^\circ = -407.777 - 1.580\times10^{-3}T\ln T - 0.624\times10^{-6}T^2 + 390.200T^{-1} + 93.482\times10^{-3}T$

2000-2327 K: $\Delta Hf^\circ = -405.772 - 0.085\times10^{-3}T + 1.066\times10^{-6}T^2 - 96.800T^{-1}$

$\Delta Gf^\circ = -405.772 + 0.085\times10^{-3}T\ln T - 1.066\times10^{-6}T^2 - 48.400T^{-1} + 80.816\times10^{-3}T$

2327-2500 K: $\Delta Hf^\circ = -414.066 + 18.310\times10^{-3}T - 0.314\times10^{-6}T^2 - 945.000T^{-1}$

$\Delta Gf^\circ = -414.066 - 18.310\times10^{-3}T\ln T + 0.314\times10^{-6}T^2 - 472.500T^{-1} + 223.853\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (36). Data for $Al_2O_3(c)$ from Ditmars (48). Liquid data based on Barkhatov (10) and Shpil'rain (200).

$Al_2O_3(\gamma)$

Dialuminum Trioxide, γ-Alumina

[Formation: $2Al(c,l) + 1.5O_2(g) = Al_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	19.773	12.500	12.500	0	-396.000	-373.770	273.977
300	19.873	12.623	12.500	.037	-396.005	-373.632	272.187
400	24.044	18.964	13.337	2.251	-396.051	-366.159	200.057
500	26.558	24.621	15.039	4.791	-395.856	-358.704	156.787
600	28.163	29.615	17.062	7.532	-395.549	-351.299	127.959
700	29.259	34.043	19.176	10.407	-395.205	-343.949	107.384
800	30.063	38.005	21.288	13.374	-394.874	-336.654	91.968
900	30.695	41.584	23.347	16.413	-394.576	-329.395	79.987
933.61	30.872	42.713	24.024	17.448	-394.486	-326.963	76.538
933.61	30.872	42.713	24.024	17.448	-399.646	-326.962	76.538
1000	31.223	44.846	25.336	19.510	-399.419	-321.802	70.329
1100	31.682	47.844	27.249	22.655	-399.051	-314.059	62.397
1200	32.094	50.618	29.080	25.845	-398.651	-306.347	55.793

*Data for $Al_2O_3(\gamma)$ and other metastable forms of Al_2O_3 are divergent.

Phase change: 933.61 K, melting point of Al; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 26.869 + 5.350\times10^{-3}T - 7.726\times10^{5}T^{-2}$

$H°- H°_{298} = 26.869\times10^{-3}T + 2.675\times10^{-6}T^{2} + 7.726\times10^{2}T^{-1} - 10.840$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -400.384 + 6.840\times10^{-3}T - 1.534\times10^{-6}T^{2} + 739.600T^{-1}$

$\Delta Gf° = -400.384 - 6.840\times10^{-3}T\ln T + 1.534\times10^{-6}T^{2} + 369.800T^{-1} + 123.617\times10^{-3}T$

933.61-1200 K: $\Delta Hf° = -402.919 + 0.844\times10^{-3}T + 1.921\times10^{-6}T^{2} + 704.800T^{-1}$

$\Delta Gf° = -402.919 - 0.844\times10^{-3}T\ln T - 1.921\times10^{-6}T^{2} + 352.400T^{-1} + 88.570\times10^{-3}T$

Source: Data from Chase (32).

Am(c,l)

Americium

T, K	cal/mol•K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15*	6.178	13.023	13.023	0
300	6.183	13.061	13.024	.011
400	6.491	14.882	13.269	.645
500	6.804	16.364	13.744	1.310
600	7.122	17.632	14.289	2.006
700	7.446	18.755	14.849	2.734
800	7.775	19.770	15.401	3.495
900	8.109	20.705	15.938	4.290
923	8.187	20.911	16.060	4.477
923	7.637	21.111	16.060	4.662
1000	7.898	21.733	16.473	5.260
1100	8.249	22.503	16.988	6.067
1200	8.616	23.236	17.478	6.910
1300	8.996	23.941	17.948	7.791
1350	9.192	24.284	18.176	8.246
1350	9.500	25.321	18.176	9.646
1400	9.500	25.666	18.437	10.121
1449	9.500	25.993	18.687	10.586
1449	10.000	28.367	18.687	14.026
1500	10.000	28.713	19.022	14.536
1600	10.000	29.358	19.648	15.536
1700	10.000	29.965	20.238	16.536
1800	10.000	30.536	20.794	17.536
1900	10.000	31.077	21.321	18.536
2000	10.000	31.590	21.822	19.536

*All data except temperatures of transitions and fusion and enthalpy of fusion are estimated.

Phase changes: 923 K, α - β transition point of Am; ΔH° = 0.185 kcal/mol.
1350 K, β - γ transition point of Am; ΔH° = 1.400 kcal/mol.
1449 K, melting point of Am; ΔH° = 3.440 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-923 K: $Cp^\circ = 5.152 + 3.270\times10^{-3}T + 0.046\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.152\times10^{-3}T + 1.635\times10^{-6}T^2 - 0.046\times10^{2}T^{-1} - 1.666$

923-1350 K: $Cp^\circ = 3.040 + 4.374\times10^{-3}T + 4.775\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 3.040\times10^{-3}T + 2.187\times10^{-6}T^2 - 4.775\times10^{2}T^{-1} + 0.510$

1350-1449 K: $Cp^\circ = 9.500$

$H^\circ - H^\circ_{298} = 9.500\times10^{-3}T - 3.179$

1449-2000 K: $Cp^\circ = 10.000$

$H^\circ - H^\circ_{298} = 10.000\times10^{-3}T - 0.464$

Source: Data from Oetting (167) who estimated all data except temperatures of transitions and fusion and enthalpy of fusion.

Am(g)

Americium (ideal monatomic gas)

[Formation: Am(c,l) = Am(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^{\circ}_{298})/T$	$H°- H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	4.968	46.473	46.473	0	67.900	57.927	-42.461
300	4.968	46.503	46.473	.009	67.898	57.865	-42.154
400	4.968	47.933	46.668	.506	67.761	54.541	-29.799
500	4.968	49.041	47.035	1.003	67.593	51.255	-22.403
600	4.968	49.947	47.447	1.500	67.394	48.005	-17.486
700	4.968	50.713	47.862	1.996	67.162	44.791	-13.984
800	4.968	51.376	48.260	2.493	66.898	41.613	-11.368
900	4.968	51.961	48.639	2.990	66.600	38.470	-9.342
923	4.968	52.086	48.723	3.104	66.527	37.752	-8.939
923	4.968	52.086	48.723	3.104	66.342	37.752	-8.939
1000	4.968	52.485	48.998	3.487	66.127	35.375	-7.731
1100	4.968	52.958	49.336	3.984	65.817	32.317	-6.421
1200	4.968	53.391	49.658	4.480	65.470	29.284	-5.333
1300	4.968	53.788	49.960	4.977	65.086	26.285	-4.419
1350	4.968	53.975	50.105	5.226	64.880	24.796	-4.014
1350	4.968	53.975	50.105	5.226	63.480	24.796	-4.014
1400	4.968	54.156	50.246	5.474	63.253	23.367	-3.648
1449	4.968	54.327	50.381	5.717	63.031	21.976	-3.314
1449	4.968	54.327	50.381	5.717	59.591	21.976	-3.314
1500	4.969	54.499	50.518	5.971	59.335	20.656	-3.010
1600	4.970	54.820	50.778	6.468	58.832	18.093	-2.471
1700	4.972	55.121	51.024	6.965	58.329	15.564	-2.001
1800	4.975	55.405	51.259	7.462	57.826	13.062	-1.586
1900	4.981	55.675	51.486	7.960	57.324	10.588	-1.218
2000	4.989	55.930	51.701	8.458	56.822	8.142	-.890

Phase changes: 923 K, α - β transition point of Am; ΔH° = 0.185 kcal/mol.
1350 K, β - γ transition point of Am; ΔH° = 1.400 kcal/mol.
1449 K, melting point of Am; ΔH° = 3.440 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.968$

$H°- H^{\circ}_{298} = 4.968\times10^{-3}T - 1.481$

Formation equations (kcal/mol):

298.15-923 K: $\Delta Hf° = 68.085 - 0.184\times10^{-3}T - 1.635\times10^{-6}T^2 + 4.600T^{-1}$

$\Delta Gf° = 68.085 + 0.184\times10^{-3}T\ln T + 1.635\times10^{-6}T^2 + 2.300T^{-1} - 35.631\times10^{-3}T$

923-1350 K: $\Delta Hf° = 65.908 + 1.928\times10^{-3}T - 2.187\times10^{-6}T^2 + 477.500T^{-1}$

$\Delta Gf° = 65.908 - 1.928\times10^{-3}T\ln T + 2.187\times10^{-6}T^2 + 238.750T^{-1} - 19.640\times10^{-3}T$

1350-1449 K: $\Delta Hf° = 69.597 - 4.532\times10^{-3}T$

$\Delta Gf° = 69.597 + 4.532\times10^{-3}T\ln T - 65.852\times10^{-3}T$

1449-2000 K: $\Delta Hf° = 66.882 - 5.032\times10^{-3}T$

$\Delta Gf° = 66.882 + 5.032\times10^{-3}T\ln T - 67.618\times10^{-3}T$

Source: Data from Oetting (167).

Ar(g)

Argon

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	4.968	36.983	36.983	0
300	4.968	37.013	36.983	.009
400	4.968	38.443	37.178	.506
500	4.968	39.551	37.545	1.003
600	4.968	40.457	37.957	1.500
700	4.968	41.223	38.372	1.996
800	4.968	41.886	38.770	2.493
900	4.968	42.471	39.149	2.990
1000	4.968	42.995	39.508	3.487
1100	4.968	43.468	39.846	3.984
1200	4.968	43.900	40.167	4.480
1300	4.968	44.298	40.470	4.977
1400	4.968	44.666	40.756	5.474
1500	4.968	45.009	41.028	5.971
1600	4.968	45.330	41.288	6.468
1700	4.968	45.631	41.535	6.964
1800	4.968	45.915	41.770	7.461
1900	4.968	46.183	41.995	7.958
2000	4.968	46.438	42.210	8.455
2100	4.968	46.681	42.418	8.952
2200	4.968	46.912	42.617	9.448
2300	4.968	47.133	42.809	9.945
2400	4.968	47.344	42.993	10.442
2500	4.968	47.547	43.171	10.939
2600	4.968	47.742	43.344	11.436
2700	4.968	47.929	43.510	11.932
2800	4.968	48.110	43.671	12.429
2900	4.968	48.284	43.827	12.926
3000	4.968	48.453	43.979	13.423

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 4.968$

$H^\circ - H^\circ_{298} = 4.968 \times 10^{-3} T - 1.481$

Source: Data from JANAF (52).

$As[\alpha,1/4As_4(g)]$

Arsenic

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.892	8.534	8.534	0
300	5.894	8.570	8.534	.011
400	6.068	10.295	8.767	.611
500	6.201	11.664	9.216	1.224
600	6.334	12.806	9.721	1.851
700	6.466	13.792	10.233	2.491
800	6.599	14.664	10.734	3.144
876	6.700	15.265	11.099	3.649
876	4.923	24.750	11.099	11.958
900	4.926	24.883	11.465	12.076
1000	4.934	25.402	12.833	12.569
1100	4.940	25.873	13.998	13.063
1200	4.944	26.303	15.005	13.557

Phase change: 876 K, sublimation point of As(c) to $As_4(g)$; ΔH° = 33.235 kcal/mol of $As_4(g)$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-876 K: $Cp^\circ = 5.691 + 1.142\times10^{-3}T - 0.124\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.691\times10^{-3}T + 0.571\times10^{-6}T^2 + 0.124\times10^{2}T^{-1} - 1.789$

876-1200 K: $Cp^\circ = 4.828 + 0.094\times10^{-3}T + 0.091\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.828\times10^{-3}T + 0.047\times10^{-6}T^2 - 0.091\times10^{2}T^{-1} + 7.703$

Source: Data from Hultgren (99).

As(g)

Arsenic (ideal monatomic gas)

[Formation: $As[c,1/4As_4(g)] = As(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^{\circ}_{298})/T$	$H°-H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	4.968	41.611	41.611	0	72.120	62.258	-45.636
300	4.968	41.642	41.612	.009	72.118	62.196	-45.309
400	4.968	43.071	41.806	.506	72.015	58.905	-32.184
500	4.968	44.179	42.173	1.003	71.899	55.642	-24.321
600	4.968	45.085	42.585	1.500	71.769	52.402	-19.087
700	4.968	45.851	43.000	1.996	71.625	49.184	-15.356
800	4.968	46.514	43.398	2.493	71.469	45.989	-12.563
876	4.968	46.966	43.689	2.871	71.342	43.572	-10.870
876	4.968	46.966	43.689	2.871	63.033	43.572	-10.870
900	4.968	47.100	43.778	2.990	63.034	43.039	-10.451
1000	4.968	47.623	44.136	3.487	63.038	40.817	-8.920
1100	4.969	48.097	44.476	3.983	63.040	38.594	-7.668
1200	4.970	48.529	44.796	4.480	63.043	36.372	-6.624

Phase change: 876 K, sublimation point of As(c) to $As_4(g)$; $\Delta H° = 33.235$ kcal/mol of $As_4(g)$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 4.968$

$H°-H^{\circ}_{298} = 4.968\times10^{-3}T - 1.481$

Formation equations (kcal/mol):

298.15-876 K: $\Delta Hf° = 72.428 - 0.723\times10^{-3}T - 0.571\times10^{-6}T^2 - 12.400T^{-1}$

$\Delta Gf° = 72.428 + 0.723\times10^{-3}T\ln T + 0.571\times10^{-6}T^2 - 6.200T^{-1} - 38.330\times10^{-3}T$

876-1200 K: $\Delta Hf° = 62.936 + 0.140\times10^{-3}T - 0.047\times10^{-6}T^2 + 9.100T^{-1}$

$\Delta Gf° = 62.936 - 0.140\times10^{-3}T\ln T + 0.047\times10^{-6}T^2 + 4.550T^{-1} - 21.202\times10^{-3}T$

Source: Data from Hultgren (99).

$As_2(g)$

Arsenic (ideal diatomic gas)

[Formation: $2As[c,1/4As_4(g)] = As_2(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.366	57.546	57.546	0	52.820	40.751	-29.871
300	8.368	57.598	57.546	.016	52.814	40.677	-29.633
400	8.594	60.040	57.875	.866	52.464	36.684	-20.043
500	8.710	61.972	58.508	1.732	52.104	32.782	-14.329
600	8.778	63.566	59.223	2.606	51.724	28.952	-10.545
700	8.820	64.922	59.942	3.486	51.324	25.187	-7.864
800	8.848	66.102	60.639	4.370	50.902	21.483	-5.869
876	8.863	66.906	61.149	5.043	50.565	18.700	-4.665
876	8.863	66.906	61.149	5.043	33.947	18.700	-4.665
900	8.868	67.146	61.306	5.256	33.924	18.282	-4.439
1000	8.882	68.080	61.938	6.142	33.824	16.548	-3.617
1100	8.892	68.928	62.535	7.032	33.726	14.826	-2.946
1200	8.900	69.702	63.102	7.920	33.626	13.111	-2.388

Phase change: 876 K, sublimation point of As(c) to $As_4(g)$; $\Delta H° = 33.235$ kcal/mol of $As_4(g)$.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 8.857 + 0.074\times10^{-3}T - 0.456\times10^{5}T^{-2}$

$H°- H°_{298} = 8.857\times10^{-3}T + 0.037\times10^{-6}T^2 + 0.456\times10^{2}T^{-1} - 2.797$

Formation equations (kcal/mol):

298.15-876 K: $\Delta Hf° = 53.601 - 2.525\times10^{-3}T - 1.105\times10^{-6}T^2 + 20.800T^{-1}$

$\Delta Gf° = 53.601 + 2.525\times10^{-3}T\ln T + 1.105\times10^{-6}T^2 + 10.400T^{-1} - 57.931\times10^{-3}T$

876-1200 K: $\Delta Hf° = 34.618 - 0.799\times10^{-3}T - 0.057\times10^{-6}T^2 + 63.800T^{-1}$

$\Delta Gf° = 34.618 + 0.799\times10^{-3}T\ln T + 0.057\times10^{-6}T^2 + 31.900T^{-1} - 23.677\times10^{-3}T$

Source: Data from Hultgren (99).

$As_3(g)$

Arsenic (ideal triatomic gas)

[Formation: $3As[c,1/4As_4(g)] = As_3(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	14.112	74.121	74.121	0	62.480	48.014	-35.195
300	14.118	74.208	74.121	.026	62.473	47.924	-34.912
400	14.439	78.321	74.684	1.455	62.102	43.128	-23.564
500	14.601	81.561	75.741	2.910	61.718	38.434	-16.799
600	14.691	84.231	76.941	4.374	61.301	33.813	-12.316
700	14.745	86.502	78.149	5.847	60.854	29.266	-9.137
800	14.781	88.473	79.319	7.323	60.371	24.786	-6.771
876	14.802	89.816	80.174	8.447	59.980	21.417	-5.343
876	14.802	89.816	80.174	8.447	35.053	21.417	-5.343
900	14.808	90.216	80.436	8.802	35.054	21.044	-5.110
1000	14.826	91.776	81.492	10.284	35.057	19.487	-4.259
1100	14.838	93.189	82.493	11.766	35.057	17.930	-3.562
1200	14.850	94.482	83.440	13.251	35.060	16.372	-2.982

*All data except enthalpy of formation at 298 K estimated.

Phase change: 876 K, sublimation point of As(c) to $As_4(g)$; $\Delta H°$ = 33.235 kcal/mol of $As_4(g)$.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 14.822 + 0.070\times10^{-3}T - 0.650\times10^{5}T^{-2}$

$H°- H°_{298} = 14.822\times10^{-3}T + 0.035\times10^{-6}T^{2} + 0.650\times10^{2}T^{-1} - 4.640$

Formation equations (kcal/mol):

298.15-876 K: $\Delta Hf° = 63.207 - 2.251\times10^{-3}T - 1.678\times10^{-6}T^{2} + 27.800T^{-1}$

$\Delta Gf° = 63.207 + 2.251\times10^{-3}T\ln T + 1.678\times10^{-6}T^{2} + 13.900T^{-1} - 64.439\times10^{-3}T$

876-1200 K: $\Delta Hf° = 34.732 + 0.338\times10^{-3}T - 0.106\times10^{-6}T^{2} + 92.300T^{-1}$

$\Delta Gf° = 34.732 - 0.338\times10^{-3}T\ln T + 0.106\times10^{-6}T^{2} + 46.150T^{-1} - 13.057\times10^{-3}T$

Source: Data from Hultgren (99) who estimated all except enthalpy of formation at 298 K.

$As_4(g)$

Arsenic (ideal tetratomic gas)

[Formation: $4As[c,1/4As_4(g)] = As_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	18.456	78.232	78.232	0	36.640	23.493	-17.220
300	18.460	78.348	78.234	.034	36.630	23.410	-17.054
400	19.056	83.752	78.962	1.916	36.112	19.083	-10.426
500	19.340	88.036	80.364	3.836	35.580	14.890	-6.508
600	19.500	91.580	81.947	5.780	35.016	10.802	-3.935
700	19.596	94.592	83.546	7.732	34.408	6.811	-2.127
800	19.660	97.212	85.092	9.696	33.760	2.915	-.796
876	19.693	99.000	86.224	11.191	33.235	0	0
876	19.693	99.000	86.224	11.191	0	0	0
900	19.704	99.532	86.572	11.664	0	0	0
1000	19.736	101.608	87.972	13.636	0	0	0
1100	19.760	103.492	89.299	15.612	0	0	0
1200	19.776	105.212	90.555	17.588	0	0	0

Phase change: 876 K, sublimation point of As(c) to $As_4(g)$; $\Delta H°$ = 33.235 kcal/mol of $As_4(g)$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 19.754 + 0.110\times10^{-3}T - 1.183\times10^{5}T^{-2}$

$H°- H°_{298} = 19.754\times10^{-3}T + 0.055\times10^{-6}T^{2} + 1.183\times10^{2}T^{-1} - 6.291$

Formation equations (kcal/mol):

298.15-876 K: $\Delta Hf° = 37.505 - 3.010\times10^{-3}T - 2.229\times10^{-6}T^{2} + 68.700T^{-1}$

$\Delta Gf° = 37.505 + 3.010\times10^{-3}T\ln T + 2.229\times10^{-6}T^{2} + 34.350T^{-1} - 65.198\times10^{-3}T$

876-1200 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Source: Data from Hultgren (99).

As_2O_3(cubic)

Diarsenic Trioxide, Arsenolite

[Formation: $2As(c) + 1.5O_2(g) = As_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.155	25.672	25.672	0	-157.020	-137.669	100.913
300	23.225	25.815	25.672	.043	-157.019	-137.549	100.203
350	24.896	29.526	25.960	1.248	-156.940	-134.309	83.866
400*	26.269	32.943	26.623	2.528	-156.799	-131.086	71.621
450	27.501	36.109	27.505	3.872	-156.607	-127.881	62.107
500	28.654	39.066	28.514	5.276	-156.373	-124.701	54.506
550	29.713	41.848	29.601	6.736	-156.099	-121.548	48.298
551	29.732	41.902	29.623	6.766	-156.093	-121.485	48.185

*Data above 360 K estimated.

Phase change: 551 K, melting point of As_2O_3(cubic).

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-551 K: $Cp° = 21.045 + 17.368\times10^{-3}T - 2.728\times10^{5}T^{-2}$

$H°- H°_{298} = 21.045\times10^{-3}T + 8.684\times10^{-6}T^2 + 2.728\times10^{2}T^{-1} - 7.961$

Formation equations (kcal/mol):

298.15-551 K: $\Delta Hf° = -157.875 - 1.182\times10^{-3}T + 6.788\times10^{-6}T^2 + 180.200T^{-1}$

$\Delta Gf° = -157.875 + 1.182\times10^{-3}T\ln T - 6.788\times10^{-6}T^2 + 90.100T^{-1} + 62.048\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities (to 360 K) and entropy at 298 K from Chang (29). Data above 360 K estimated.

As_2O_3(monoclinic)

Diarsenic Trioxide, Claudetite

[Formation: $2As(c) + 1.5O_2(g) = As_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.178	27.087	27.087	0	-156.500	-137.571	100.841
300	23.245	27.231	27.088	.043	-156.499	-137.454	100.134
350	24.829	30.938	27.378	1.246	-156.422	-134.286	83.851
400*	26.092	34.339	28.037	2.521	-156.286	-131.131	71.646
450	27.181	37.476	28.914	3.853	-156.106	-127.995	62.162
500	28.184	40.392	29.918	5.237	-155.892	-124.883	54.586
550	29.118	43.123	30.996	6.670	-155.645	-121.795	48.396
585	29.700	44.937	31.775	7.700	-155.454	-119.646	44.698

*Data above 360 K estimated.

Phase change: 585 K, melting point of As_2O_3(monoclinic).

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-585 K: $Cp° = 22.397 + 13.978\times10^{-3}T - 3.010\times10^{5}T^{-2}$

$H°- H°_{298} = 22.397\times10^{-3}T + 6.989\times10^{-6}T^{2} + 3.010\times10^{2}T^{-1} - 8.309$

Formation equations (kcal/mol):

298.15-585 K: $\Delta Hf° = -157.702 + 0.170\times10^{-3}T + 5.093\times10^{-6}T^{2} + 208.400T^{-1}$

$\Delta Gf° = -157.702 - 0.170\times10^{-3}T\ln T - 5.093\times10^{-6}T^{2} + 104.200T^{-1} + 68.836\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities (to 360 K) and entropy at 298 K from Chang (29). Data above 360 K estimated.

$As_2O_5(c)$

Diarsenic Pentoxide

[Formation: $2As(c) + 2.5O_2(g) = As_2O_5(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	27.853	25.200	25.200	0	-221.050	-186.947	137.034
300*	27.955	25.373	25.200	.052	-221.053	-186.736	136.035
400	32.671	34.095	26.358	3.095	-220.984	-175.296	95.776
500	36.320	41.792	28.690	6.551	-220.582	-163.913	71.645
600	39.317	48.687	31.459	10.337	-219.938	-152.637	55.597

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 24.102 + 27.514\times10^{-3}T - 3.958\times10^{5}T^{-2}$

$H°- H°_{298} = 24.102\times10^{-3}T + 13.757\times10^{-6}T^{2} + 3.958\times10^{2}T^{-1} - 9.736$

Formation equations (kcal/mol):

298.15-600 K: $\Delta Hf° = -221.328 - 5.355\times10^{-3}T + 11.358\times10^{-6}T^{2} + 258.000T^{-1}$

$\Delta Gf° = -221.328 + 5.355\times10^{-3}T\ln T - 1.358\times10^{-6}T^{2} + 129.000T^{-1} + 86.739\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities and entropy at 298 K from Anderson (1). Data above 298 K estimated.

$As_4O_6(g)$

Tetrarsenic Hexoxide (ideal gas)

[Formation: $4As[c,1/4As_4(g)] + 3O_2(g) = As_4O_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	41.490	97.810	97.810	0	-285.910	-261.062	191.361
300.00	41.610	98.070	97.813	.077	-285.916	-260.909	190.070
400.00	46.560	110.790	99.518	4.509	-286.014	-252.550	137.985
500.00	49.390	121.510	102.874	9.318	-285.850	-244.195	106.736
600.00	51.110	130.670	106.753	14.350	-285.591	-235.884	85.920
700.00	52.230	138.640	110.753	19.521	-285.314	-227.623	71.066
800.00	52.980	145.670	114.691	24.783	-285.058	-219.405	59.938
876.00	53.383	150.495	117.589	28.826	-284.887	-213.180	53.185
876.00	53.383	150.495	117.589	28.826	-318.122	-213.180	53.185
900.00	53.510	151.940	118.486	30.109	-317.902	-210.308	51.069
1000.00	53.900	157.600	122.119	35.481	-316.983	-198.405	43.361

Phase change: 876 K, sublimation point of As(c) to $As_4(g)$; $\Delta H° = 33.235$ kcal/mol of $As_4(g)$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 50.862 + 4.438\times10^{-3}T - 9.507\times10^{5}T^{-2}$

$H°-H°_{298} = 50.862\times10^{-3}T + 2.219\times10^{-6}T^{2} + 9.507\times10^{2}T^{-1} - 18.550$

Formation equations (kcal/mol):

298.15-876 K: $\Delta Hf° = -290.248 + 6.408\times10^{-3}T - 1.574\times10^{-6}T^{2} + 765.500T^{-1}$

$\Delta Gf° = -290.248 - 6.408\times10^{-3}T\ln T + 1.574\times10^{-6}T^{2} + 382.750T^{-1} + 129.626\times10^{-3}T$

876-1000 K: $\Delta Hf° = -328.215 + 9.860\times10^{-3}T + 0.522\times10^{-6}T^{2} + 851.500T^{-1}$

$\Delta Gf° = -328.215 - 9.860\times10^{-3}T\ln T - 0.522\times10^{-6}T^{2} + 425.750T^{-1} + 198.136\times10^{-3}T$

Source: Data from Behrens (13).

Au(c,1)

Gold

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.075	11.330	11.330	0
300	6.078	11.368	11.331	.011
400	6.187	13.133	11.571	.625
500	6.281	14.524	12.028	1.248
600	6.397	15.679	12.542	1.882
700	6.510	16.674	13.063	2.528
800	6.597	17.549	13.570	3.183
900	6.662	18.330	14.057	3.846
1000	6.742	19.036	14.520	4.516
1100	6.904	19.685	14.960	5.197
1200	7.254	20.299	15.380	5.903
1300	7.932	20.903	15.781	6.659
1337.58	8.306	21.134	15.928	6.964
1337.58	7.972	23.345	15.928	9.921
1400	7.972	23.709	16.267	10.419
1500	7.972	24.259	16.782	11.216
1600	7.972	24.773	17.265	12.013
1700	7.972	25.257	17.722	12.810
1800	7.972	25.712	18.153	13.607
1900	7.972	26.143	18.561	14.405
2000	7.972	26.552	18.951	15.202

Phase changes: 1337.58 K, melting point of Au; ΔH° = 2.957 kcal/mol.
3130 K, boiling point of Au; ΔH° = 80.0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1337.58 K:

$$Cp^\circ = 5.409 + 1.520\times10^{-3}T + 0.188\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 5.409\times10^{-3}T + 0.760\times10^{-6}T^2 - 0.188\times10^{2}T^{-1} - 1.617$$

1337.58-2000 K:

$$Cp^\circ = 7.972$$

$$H^\circ - H^\circ_{298} = 7.972\times10^{-3}T - 0.742$$

Sources: Low-temperature heat capacities and entropy at 298 K from Furukawa (73). High-temperature data based on Hultgren (99), Tester (219), and Plaza (185). Data corrected to IPTS-68.

Au(g)

Gold (ideal monatomic gas)

[Formation: Au(c,l) = Au(g)]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^{\circ}_{298})/T$	$H°- H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	4.968	43.116	43.116	0	87.500	78.023	-57.192
300	4.968	43.147	43.117	.009	87.498	77.964	-56.796
400	4.968	44.576	43.311	.506	87.381	74.804	-40.870
500	4.968	45.684	43.678	1.003	87.255	71.675	-31.329
600	4.968	46.590	44.090	1.500	87.118	68.571	-24.977
700	4.968	47.356	44.505	1.996	86.968	65.491	-20.447
800	4.968	48.019	44.903	2.493	86.810	62.434	-17.056
900	4.969	48.605	45.283	2.990	86.644	59.396	-14.423
1000	4.970	49.128	45.641	3.487	86.471	56.379	-12.321
1100	4.973	49.602	45.980	3.984	86.287	53.378	-10.605
1200	4.980	50.035	46.300	4.482	86.079	50.396	-9.178
1300	4.992	50.434	46.603	4.980	85.821	47.431	-7.974
1337.58	4.999	50.576	46.713	5.168	85.704	46.323	-7.569
1337.58	4.999	50.576	46.713	5.168	82.747	46.323	-7.569
1400	5.011	50.805	46.891	5.480	82.561	44.627	-6.966
1500	5.038	51.151	47.162	5.983	82.267	41.929	-6.109
1600	5.075	51.477	47.422	6.488	81.975	39.249	-5.361
1700	5.121	51.786	47.670	6.998	81.688	36.589	-4.704
1800	5.178	52.081	47.907	7.513	81.406	33.942	-4.121
1900	5.245	52.362	48.134	8.034	81.129	31.313	-3.602
2000	5.321	52.633	48.352	8.562	80.860	28.698	-3.136

Phase change: 1337.58 K, melting point of Au; $\Delta H° = 2.957$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.899 + 0.092\times10^{-3}T + 0.037\times10^{5}T^{-2}$

$H°- H^{\circ}_{298} = 4.899\times10^{-3}T + 0.046\times10^{-6}T^{2} - 0.037\times10^{2}T^{-1} - 1.452$

Formation equations (kcal/mol):

298.15-1337.58K: $\Delta Hf° = 87.665 - 0.510\times10^{-3}T - 0.714\times10^{-6}T^{2} + 15.100T^{-1}$

$\Delta Gf° = 87.665 + 0.510\times10^{-3}T\ln T + 0.714\times10^{-6}T^{2} + 7.550T^{-1} - 35.543\times10^{-3}T$

1337.58-2000 K: $\Delta Hf° = 86.790 - 3.073\times10^{-3}T + 0.046\times10^{-6}T^{2} - 3.700T^{-1}$

$\Delta Gf° = 86.790 + 3.073\times10^{-3}T\ln T - 0.046\times10^{-6}T^{2} - 1.850T^{-1} - 52.317\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). All other data from Hilsenrath (94).

B(β)

Boron

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	2.650	1.410	1.410	0
300	2.660	1.430	1.413	.005
400	3.660	2.330	1.525	.322
500	4.440	3.240	1.782	.729
600	4.990	4.100	2.093	1.204
700	5.340	4.900	2.440	1.722
800	5.580	5.630	2.795	2.268
900	5.780	6.300	3.148	2.837
1000	5.960	6.920	3.495	3.425
1100	6.120	7.490	3.827	4.029
1200	6.260	8.030	4.157	4.648
1300	6.410	8.540	4.477	5.282
1400	6.560	9.020	4.784	5.930
1500	6.710	9.480	5.085	6.593
1600	6.850	9.910	5.366	7.271
1700	6.990	10.330	5.646	7.963
1800	7.130	10.740	5.924	8.669
1900	7.270	11.130	6.188	9.389
2000	7.410	11.500	6.438	10.123

Phase changes: 2300 K, melting point of B; ΔH° = 12.0 kcal/mol.
4275 K, boiling point of B; ΔH° = 117.0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15–2000 K: $Cp^\circ = 4.577 + 1.508\times10^{-3}T - 2.113\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.577\times10^{-3}T + 0.754\times10^{-6}T^2 + 2.113\times10^{2}T^{-1} - 2.140$

Sources: Entropy at 298 K from CODATA (36). All other data from Hultgren (99).

B(g)

Boron (ideal monatomic gas)

[Formation: B(c) = B(g)]

T, K	cal/mol°K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^{\circ}_{298})/T$	$H°- H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	4.971	36.649	36.649	0	132.800	122.293	-89.642
300	4.971	36.680	36.650	.009	132.804	122.229	-89.043
400	4.970	38.110	36.845	.506	132.984	118.672	-64.839
500	4.969	39.219	37.213	1.003	133.074	115.085	-50.303
600	4.969	40.125	37.625	1.500	133.096	111.481	-40.606
700	4.969	40.891	38.038	1.997	133.075	107.881	-33.682
800	4.969	41.554	38.437	2.494	133.026	104.287	-28.489
900	4.968	42.139	38.816	2.991	132.954	100.699	-24.453
1000	4.968	42.663	39.176	3.487	132.862	97.119	-21.225
1100	4.968	43.136	39.514	3.984	132.755	93.544	-18.585
1200	4.968	43.569	39.835	4.481	132.633	89.986	-16.389
1300	4.968	43.966	40.137	4.978	132.496	86.442	-14.532
1400	4.968	44.335	40.424	5.475	132.345	82.904	-12.942
1500	4.968	44.677	40.696	5.972	132.179	79.384	-11.566
1600	4.968	44.998	40.956	6.468	131.997	75.856	-10.361
1700	4.968	45.299	41.202	6.965	131.802	72.355	-9.302
1800	4.968	45.583	41.437	7.462	131.593	68.876	-8.363
1900	4.968	45.852	41.663	7.959	131.370	65.398	-7.522
2000	4.968	46.107	41.879	8.456	131.133	61.919	-6.766

Heat capacity (cal/mol°K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.968 + 0.003\times10^{5}T^{-2}$

$H°- H^{\circ}_{298} = 4.968\times10^{-3}T - 0.003\times10^{2}T^{-1} - 1.480$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 133.460 + 0.391\times10^{-3}T - 0.754\times10^{-6}T^{2} - 211.600T^{-1}$

$\Delta Gf° = 133.460 - 0.391\times10^{-3}T\ln T + 0.754\times10^{-6}T^{2} - 105.800T^{-1} - 34.260\times10^{-3}T$

Source: Data from JANAF (51).

$B_2(g)$

Boron (ideal diatomic gas)

[Formation: $2B(c) = B_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^{\circ}_{298})/T$	$H°- H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	7.301	48.228	48.228	0	198.500	184.962	-135.579
300	7.307	48.273	48.228	.014	198.504	184.880	-134.683
400	7.667	50.425	48.520	.762	198.618	180.312	-98.517
500	7.976	52.170	49.080	1.545	198.587	175.742	-76.816
600	8.212	53.646	49.721	2.355	198.447	171.179	-62.351
700	8.388	54.926	50.375	3.186	198.242	166.654	-52.031
800	8.521	56.055	51.016	4.031	197.995	162.159	-44.299
900	8.623	57.065	51.633	4.889	197.715	157.697	-38.293
1000	8.703	57.978	52.223	5.755	197.405	153.267	-33.496
1100	8.767	58.811	52.785	6.629	197.071	148.857	-29.575
1200	8.820	59.576	53.319	7.508	196.712	144.493	-26.315
1300	8.865	60.284	53.828	8.393	196.329	140.164	-23.563
1400	8.902	60.942	54.313	9.281	195.921	135.858	-21.208
1500	8.935	61.557	54.775	10.173	195.487	131.591	-19.173
1600	8.964	62.135	55.217	11.068	195.026	127.322	-17.391
1700	8.991	62.679	55.640	11.966	194.540	123.108	-15.826
1800	9.014	63.194	56.046	12.866	194.028	118.943	-14.441
1900	9.036	63.682	56.435	13.769	193.491	114.789	-13.204
2000	9.056	64.146	56.810	14.673	192.927	110.635	-12.089

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.053 + 0.638\times10^{-3}T - 0.838\times10^{5}T^{-2}$

$H°- H^{\circ}_{298} = 8.053\times10^{-3}T + 0.319\times10^{-6}T^{2} + 0.838\times10^{2}T^{-1} - 2.710$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 200.070 - 1.101\times10^{-3}T - 1.189\times10^{-6}T^{2} - 338.800T^{-1}$

$\Delta Gf° = 200.070 + 1.101\times10^{-3}T\ln T + 1.189\times10^{-6}T^{2} - 169.400T^{-1} - 55.397\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from JANAF (51).

BO(g)

Boron Oxide (ideal gas)

[Formation: $B(c) + \frac{1}{2}O_2(g) = BO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	6.978	48.604	48.604	0	6.000	-0.765	0.561
300	6.979	48.647	48.604	.013	6.002	-.806	.587
400	7.068	50.665	48.878	.715	6.032	-3.085	1.685
500	7.230	52.259	49.401	1.429	5.973	-5.356	2.341
600	7.427	53.594	49.991	2.162	5.853	-7.614	2.773
700	7.627	54.754	50.591	2.914	5.699	-9.846	3.074
800	7.810	55.785	51.176	3.687	5.527	-12.053	3.293
900	7.971	56.714	51.741	4.476	5.339	-14.240	3.458
1000	8.108	57.561	52.281	5.280	5.142	-16.404	3.585
1100	8.225	58.340	52.797	6.097	4.936	-18.555	3.686
1200	8.324	59.060	53.290	6.924	4.719	-20.680	3.766
1300	8.408	59.729	53.759	7.761	4.495	-22.783	3.830
1400	8.480	60.355	54.208	8.606	4.259	-24.872	3.883
1500	8.542	60.942	54.637	9.457	4.012	-26.941	3.925
1600	8.595	61.495	55.049	10.314	3.753	-29.008	3.962
1700	8.641	62.018	55.444	11.175	3.481	-31.048	3.991
1800	8.682	62.513	55.823	12.042	3.198	-33.058	4.014
1900	8.717	62.983	56.187	12.912	2.901	-35.062	4.033
2000	8.749	63.431	56.539	13.785	2.590	-37.065	4.050

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.733 + 1.244\times10^{-3}T - 0.112\times10^{5}T^{-2}$

$H°-H°_{298} = 6.733\times10^{-3}T + 0.622\times10^{-6}T^{2} + 0.112\times10^{2}T^{-1} - 2.100$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 7.216 - 1.459\times10^{-3}T - 0.383\times10^{-6}T^{2} - 222.700T^{-1}$

$\Delta Gf° = 7.216 + 1.459\times10^{-3}T\ln T + 0.383\times10^{-6}T^{2} - 111.350T^{-1} - 33.945\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from JANAF (51).

$BO_2(g)$

Boron Dioxide (ideal gas)

[Formation: $B(c) + O_2(g) = BO_2(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.343	54.900	54.900	0	-71.800	-73.137	53.610
300	10.363	54.964	54.901	.019	-71.799	-73.145	53.285
400	11.351	58.085	55.320	1.106	-71.739	-73.605	40.215
500	12.137	60.706	56.140	2.283	-71.700	-74.073	32.377
600	12.730	62.974	57.096	3.527	-71.686	-74.552	27.155
700	13.171	64.971	58.080	4.824	-71.685	-75.028	23.424
800	13.501	66.752	59.055	6.158	-71.695	-75.505	20.627
900	13.750	68.358	60.001	7.521	-71.715	-75.980	18.450
1000	13.942	69.817	60.911	8.906	-71.745	-76.452	16.708
1100	14.091	71.153	61.782	10.308	-71.786	-76.926	15.284
1200	14.209	72.384	62.615	11.723	-71.838	-77.389	14.094
1300	14.304	73.525	63.410	13.149	-71.902	-77.846	13.087
1400	14.381	74.588	64.172	14.583	-71.980	-78.301	12.223
1500	14.444	75.583	64.900	16.025	-72.071	-78.746	11.473
1600	14.497	76.517	65.597	17.472	-72.179	-79.200	10.818
1700	14.541	77.397	66.265	18.924	-72.301	-79.633	10.237
1800	14.579	78.229	66.907	20.380	-72.439	-80.048	9.719
1900	14.611	79.018	67.524	21.839	-72.594	-80.466	9.256
2000	14.639	79.768	68.117	23.302	-72.764	-80.888	8.839

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.306 + 1.590\times10^{-3}T - 2.166\times10^{5}T^{-2}$

$H°- H°_{298} = 12.306\times10^{-3}T + 0.795\times10^{-6}T^{2} + 2.166\times10^{2}T^{-1} - 4.466$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -71.774 + 0.499\times10^{-3}T - 0.462\times10^{-6}T^{2} - 39.900T^{-1}$

$\Delta Gf° = -71.774 - 0.499\times10^{-3}T\ln T + 0.462\times10^{-6}T^{2} - 19.950T^{-1} - 1.643\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from JANAF (51).

$B_2O(g)$

Diboron Oxide (ideal gas)

[Formation: $2B(c) + 0.5O_2(g) = B_2O(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.180	54.405	54.405	0	23.000	14.925	-10.940
300	9.193	54.462	54.405	.017	23.000	14.877	-10.838
400	9.903	57.205	54.775	.972	22.966	12.166	-6.647
500	10.556	59.486	55.494	1.996	22.811	9.488	-4.147
600	11.121	61.462	56.329	3.080	22.567	6.839	-2.491
700	11.588	63.213	57.189	4.217	22.280	4.244	-1.325
800	11.966	64.786	58.042	5.395	21.967	1.690	-.462
900	12.269	66.213	58.872	6.607	21.634	-0.825	.200
1000	12.514	67.519	59.672	7.847	21.284	-3.300	.721
1100	12.712	68.721	60.441	9.108	20.918	-5.753	1.143
1200	12.873	69.835	61.178	10.388	20.536	-8.158	1.486
1300	13.005	70.870	61.884	11.682	20.133	-10.525	1.769
1400	13.115	71.838	62.561	12.988	19.711	-12.869	2.009
1500	13.206	72.746	63.210	14.304	19.267	-15.173	2.211
1600	13.284	73.601	63.833	15.629	18.797	-17.477	2.387
1700	13.349	74.409	64.432	16.961	18.304	-19.728	2.536
1800	13.405	75.173	65.007	18.298	17.785	-21.927	2.662
1900	13.450	75.899	65.562	19.641	17.241	-24.115	2.774
2000	13.495	76.590	66.095	20.989	16.672	-26.302	2.874

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.353 + 2.026\times10^{-3}T - 1.580\times10^{5}T^{-2}$

$H°- H°_{298} = 10.353\times10^{-3}T + 1.013\times10^{-6}T^{2} + 1.580\times10^{2}T^{-1} - 3.707$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 24.750 - 2.416\times10^{-3}T - 0.746\times10^{-6}T^{2} - 287.200T^{-1}$

$\Delta Gf° = 24.750 + 2.416\times10^{-3}T\ln T + 0.746\times10^{-6}T^{2} - 143.600T^{-1} - 45.324\times10^{-3}T$

Source: All data from JANAF (51).

$B_2O_3(c,l)$

Diboron Trioxide

[Formation: $2B(c) + 1.5O_2(g) = B_2O_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.980	12.900	12.900	0	-304.370	-285.459	209.244
300	15.056	12.993	12.900	.028	-304.371	-285.339	207.867
400	18.631	17.839	13.537	1.721	-304.377	-278.995	152.434
500	21.337	22.300	14.850	3.725	-304.284	-272.653	119.175
600	23.453	26.385	16.437	5.969	-304.122	-266.346	97.015
700	25.157	30.132	18.129	8.402	-303.892	-260.064	81.195
723	25.502	30.952	18.525	8.985	-303.829	-258.625	78.177
723	31.800	38.891	18.525	14.725	-298.089	-258.625	78.177
800	31.800	42.109	20.643	17.173	-297.410	-254.458	69.514
900	31.800	45.855	23.241	20.353	-296.590	-249.138	60.498
1000	31.800	49.205	25.672	23.533	-295.826	-243.906	53.305
1100	31.800	52.236	27.951	26.713	-295.112	-238.761	47.437
1200	31.800	55.003	30.092	29.893	-294.443	-233.664	42.555
1300	31.800	57.548	32.107	33.073	-293.814	-228.618	38.434
1400	31.800	59.905	34.010	36.253	-293.227	-223.626	34.909
1500	31.800	62.099	35.810	39.433	-292.678	-218.667	31.859
1600	31.800	64.151	37.518	42.613	-292.169	-213.773	29.200
1700	31.800	66.079	39.142	45.793	-291.696	-208.886	26.854
1800	31.800	67.897	40.690	48.973	-291.260	-204.003	24.769

Phase change: 723 K, melting point of B_2O_3; $\Delta H° = 5.740$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-723 K: $Cp° = 14.287 + 16.964\times10^{-3}T - 3.880\times10^{5}T^{-2}$

$H°- H°_{298} = 14.287\times10^{-3}T + 8.482\times10^{-6}T^2 + 3.880\times10^{2}T^{-1} - 6.315$

723-1800 K: $Cp° = 31.800$

$H°- H°_{298} = 31.800\times10^{-3}T - 8.266$

Formation equations (kcal/mol):

298.15-723 K: $\Delta Hf° = -302.876 - 5.712\times10^{-3}T + 6.219\times10^{-6}T^2 - 102.400T^{-1}$

$\Delta Gf° = -302.876 + 5.712\times10^{-3}T\ln T - 6.219\times10^{-6}T^2 - 51.200T^{-1} + 28.304\times10^{-3}T$

723-1800 K: $\Delta Hf° = -304.828 + 11.801\times10^{-3}T - 2.263\times10^{-6}T^2 - 490.400T^{-1}$

$\Delta Gf° = -304.828 - 11.801\times10^{-3}T\ln T + 2.263\times10^{-6}T^2 - 245.200T^{-1} + 140.537\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (36). Low-temperature heat capacity based on Kelley (117) and Kerr (124). High-temperature data based on Shmidt (195).

B_2O_3(amorphous)

Diboron Trioxide

[Formation: $2B(c) + 1.5O_2(g) = B_2O_3$(amorphous)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.980	18.650	18.650	0	-299.840	-282.643	207.181
300	15.060	18.740	18.650	.028	-299.841	-282.533	205.823
400	18.630	23.590	19.288	1.721	-299.847	-276.765	151.216
500	21.340	28.050	20.600	3.725	-299.754	-270.998	118.452
600	31.800	32.980	22.228	6.451	-299.111	-265.291	96.631
700	31.800	37.880	24.121	9.631	-298.133	-259.729	81.090
723	31.800	38.910	24.577	10.363	-297.921	-258.471	78.130

Phase change: 723 K, melting point of B_2O_3.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-723 K: $Cp° = -4.534 + 53.864\times10^{-3}T + 3.071\times10^{5}T^{-2}$

$H°- H°_{298} = -4.534\times10^{-3}T + 26.932\times10^{-6}T^{2} - 3.071\times10^{2}T^{-1} - 0.012$

Formation equations (kcal/mol):

298.15-723 K: $\Delta Hf° = -292.044 - 24.533\times10^{-3}T + 24.670\times10^{-6}T^{2} - 797.500T^{-1}$

$\Delta Gf° = -292.044 + 24.533\times10^{-3}T\ln T - 24.670\times10^{-6}T^{2} - 398.750T^{-1} - 96.410\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Entropy at 298 K based on Shmidt (195) and Wagman (236). Low-temperature heat capacities from Turdakin (229). High-temperature data based on Shmidt (195).

Ba(c,l)

Barium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.713	14.918	14.918	0
300	6.724	14.960	14.920	.012
400	7.897	17.032	15.187	.738
500	10.440	19.048	15.756	1.646
582	13.010	20.823	16.344	2.607
600	8.585	21.084	16.482	2.761
700	9.833	22.492	17.241	3.676
768	10.145	23.422	17.748	4.358
800	10.084	23.835	17.983	4.682
900	9.651	24.988	18.698	5.661
1000	9.777	26.012	19.379	6.633
1002	9.778	26.032	19.392	6.653
1002	10.349	27.880	19.392	8.505
1100	10.060	28.833	20.192	9.505
1200	9.765	29.695	20.948	10.496
1300	9.700	30.473	21.652	11.467
1400*	9.700	31.191	22.307	12.437
1500	9.700	31.861	22.923	13.407
1600	9.700	32.487	23.501	14.377
1700	9.700	33.075	24.047	15.347
1800	9.700	33.629	24.564	16.317
1900	9.700	34.154	25.056	17.287
2000	9.700	34.651	25.523	18.257

*Data above 1300 K extrapolated.

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.
2171 K, boiling point of Ba; ΔH° = 33.8 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-582 K: $C_p^\circ = -9.723 + 36.500\times10^{-3}T + 4.935\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = -9.723\times10^{-3}T + 18.250\times10^{-6}T^2 - 4.935\times10^{2}T^{-1} + 2.932$

582-768 K: $C_p^\circ = 2.517 + 10.220\times10^{-3}T$

$H^\circ - H^\circ_{298} = 2.517\times10^{-3}T + 5.110\times10^{-6}T^2 - 0.589$

768-1002 K: $C_p^\circ = 10.659 - 0.962\times10^{-3}T - 0.004\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.659\times10^{-3}T - 0.481\times10^{-6}T^2 + 0.004\times10^{2}T^{-1} - 3.545$

1002-2000 K: $C_p^\circ = 6.592 + 1.298\times10^{-3}T + 24.659\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.592\times10^{-3}T + 0.649\times10^{-6}T^2 - 24.659\times10^{2}T^{-1} + 3.709$

Source: Data from Hultgren (99) who extrapolated above 1300 K by assuming constant heat capacity.

Ba(g)

Barium (ideal monatomic gas)

[Formation: Ba(c,l) = Ba(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	40.663	40.663	0	43.000	35.324	-25.893
300	4.968	40.694	40.664	.009	42.997	35.277	-25.699
400	4.968	42.123	40.858	.506	42.768	32.732	-17.883
500	4.968	43.231	41.225	1.003	42.357	30.265	-13.229
582	4.968	43.986	41.562	1.411	41.804	28.323	-10.636
600	4.968	44.137	41.637	1.500	41.739	27.907	-10.165
700	4.968	44.903	42.052	1.996	41.320	25.632	-8.003
768	4.968	45.363	42.324	2.334	40.976	24.125	-6.865
800	4.968	45.566	42.450	2.493	40.811	23.426	-6.400
900	4.970	46.152	42.830	2.990	40.329	21.281	-5.168
1000	4.976	46.675	43.188	3.487	39.854	19.191	-4.194
1002	4.976	46.685	43.195	3.497	39.844	19.150	-4.177
1002	4.976	46.685	43.195	3.497	37.992	19.150	-4.177
1100	4.991	47.150	43.526	3.986	37.481	17.332	-3.444
1200	5.022	47.586	43.848	4.486	36.990	15.521	-2.827
1300	5.079	47.990	44.151	4.991	36.524	13.752	-2.312
1400	5.171	48.369	44.438	5.503	36.066	12.017	-1.876
1500	5.307	48.731	44.713	6.027	35.620	10.315	-1.503
1600	5.496	49.079	44.975	6.566	35.189	8.642	-1.180
1700	5.743	49.419	45.226	7.128	34.781	6.996	-.899
1800	6.052	49.756	45.469	7.717	34.400	5.371	-.652
1900	6.422	50.093	45.704	8.340	34.053	3.769	-.434
2000	6.848	50.433	45.931	9.003	33.746	2.182	-.238

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.562 + 0.510\times10^{-3}T + 0.226\times10^{5}T^{-2}$

$H°- H°_{298} = 4.562\times10^{-3}T + 0.255\times10^{-6}T^{2} - 0.226\times10^{2}T^{-1} - 1.307$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = 38.761 + 14.285\times10^{-3}T - 17.995\times10^{-6}T^{2} + 470.900T^{-1}$

$\Delta Gf° = 38.761 - 14.285\times10^{-3}T\ln T + 17.995\times10^{-6}T^{2} + 235.450T^{-1} + 61.848\times10^{-3}T$

582-768 K: $\Delta Hf° = 42.282 + 2.045\times10^{-3}T - 4.855\times10^{-6}T^{2} - 22.600T^{-1}$

$\Delta Gf° = 42.282 - 2.045\times10^{-3}T\ln T + 4.855\times10^{-6}T^{2} - 11.300T^{-1} - 13.751\times10^{-3}T$

768-1002 K: $\Delta Hf° = 45.238 - 6.097\times10^{-3}T + 0.736\times10^{-6}T^{2} - 23.000T^{-1}$

$\Delta Gf° = 45.238 + 6.097\times10^{-3}T\ln T - 0.736\times10^{-6}T^{2} - 11.500T^{-1} - 67.399\times10^{-3}T$

1002-2000 K: $\Delta Hf° = 37.984 - 2.030\times10^{-3}T - 0.394\times10^{-6}T^{2} + 2443.300T^{-1}$

$\Delta Gf° = 37.984 + 2.030\times10^{-3}T\ln T + 0.394\times10^{-6}T^{2} + 1221.650T^{-1} - 34.418\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (180). All other data from Chase (31).

BaO(c)

Barium Oxide

[Formation: $Ba(c,l) + 0.5O_2(g) = BaO(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.340	16.830	16.830	0	-130.980	-124.245	91.073
300	11.353	16.900	16.830	.021	-130.977	-124.202	90.480
400	11.939	20.253	17.283	1.188	-130.891	-121.962	66.636
500	12.366	22.965	18.157	2.404	-130.949	-119.727	52.332
582	12.649	24.865	18.972	3.430	-131.193	-117.871	44.262
600	12.711	25.251	19.154	3.658	-131.188	-117.459	42.784
700	13.001	27.233	20.170	4.944	-131.205	-115.171	35.957
768	13.170	28.447	20.850	5.834	-131.268	-113.610	32.330
800	13.249	28.986	21.165	6.257	-131.298	-112.874	30.835
900	13.464	30.559	22.122	7.593	-131.347	-110.568	26.849
1000	13.653	31.987	23.038	8.949	-131.377	-108.257	23.659
1002	13.656	32.014	23.056	8.976	-131.378	-108.211	23.602
1002	13.656	32.014	23.056	8.976	-133.230	-108.211	23.602
1100	13.821	33.297	23.912	10.323	-133.294	-105.760	21.012
1200	13.974	34.506	24.745	11.713	-133.320	-103.256	18.805
1300	14.117	35.630	25.540	13.117	-133.314	-100.750	16.937
1400*	14.254	36.681	26.298	14.536	-133.298	-98.246	15.337
1500	14.391	37.670	27.025	15.968	-133.270	-95.744	13.950
1600	14.532	38.603	27.719	17.414	-133.233	-93.243	12.736
1700	14.681	39.488	28.385	18.875	-133.183	-90.744	11.666
1800	14.844	40.332	29.026	20.351	-133.121	-88.251	10.715

*Data extrapolated above 1300 K.

Phase changes: 582 K, α - β transition point of Ba; $\Delta H° = 0$ kcal/mol.
768 K, β - γ transition point of Ba; $\Delta H° = 0$ kcal/mol.
1002 K, melting point of Ba; $\Delta H° = 1.852$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 11.931 + 1.730\times10^{-3}T - 0.983\times10^{5}T^{-2}$

$H°- H°_{298} = 11.931\times10^{-3}T + 0.865\times10^{-6}T^{2} + 0.983\times10^{2}T^{-1} - 3.964$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = -136.700 + 18.039\times10^{-3}T - 17.636\times10^{-6}T^{2} + 569.200T^{-1}$

$\Delta Gf° = -136.700 - 18.039\times10^{-3}T\ln T + 17.636\times10^{-6}T^{2} + 284.600T^{-1} + 136.093\times10^{-3}T$

582-768 K: $\Delta Hf° = -133.179 + 5.799\times10^{-3}T - 4.496\times10^{-6}T^{2} + 75.700T^{-1}$

$\Delta Gf° = -133.179 - 5.799\times10^{-3}T\ln T + 4.496\times10^{-6}T^{2} + 37.850T^{-1} + 60.494\times10^{-3}T$

768-1002 K: $\Delta Hf° = -130.223 - 2.343\times10^{-3}T + 1.095\times10^{-6}T^{2} + 75.300T^{-1}$

$\Delta Gf° = -130.223 + 2.343\times10^{-3}T\ln T - 1.095\times10^{-6}T^{2} + 37.650T^{-1} + 6.846\times10^{-3}T$

1002-1800 K: $\Delta Hf° = -137.477 + 1.724\times10^{-3}T - 0.036\times10^{-6}T^{2} + 2541.600T^{-1}$

$\Delta Gf° = -137.477 - 1.724\times10^{-3}T\ln T + 0.036\times10^{-6}T^{2} + 1270.800T^{-1} + 39.827\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Fitzgibbon (63). Entropy at 298 K from Parker (180). Low-temperature heat capacities from Anderson (4). High-temperature data to 1200 K based on Lander (141). Extrapolated above 1300 K.

BaO(g)

Barium Oxide (ideal gas)

[Formation: $Ba(c,l) + 0.5O_2(g) = BaO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.863	56.249	56.249	0	-29.600	-34.617	25.375
300	7.871	56.297	56.247	.015	-29.604	-34.647	25.240
400	8.232	58.615	56.563	.821	-29.879	-36.294	19.830
500	8.457	60.478	57.166	1.656	-30.317	-37.852	16.545
582	8.575	61.772	57.725	2.355	-30.887	-39.045	14.662
600	8.601	62.034	57.851	2.510	-30.955	-39.296	14.314
700	8.698	63.367	58.546	3.375	-31.395	-40.653	12.692
768	8.744	64.177	59.010	3.968	-31.754	-41.537	11.820
800	8.766	64.534	59.224	4.248	-31.927	-41.942	11.458
900	8.816	65.569	59.871	5.128	-32.432	-43.162	10.481
1000	8.855	66.500	60.489	6.011	-32.935	-44.328	9.688
1002	8.856	66.518	60.501	6.029	-32.946	-44.351	9.673
1002	8.856	66.518	60.501	6.029	-34.798	-44.351	9.673
1100	8.885	67.346	61.075	6.898	-35.340	-45.259	8.992
1200	8.910	68.120	61.630	7.788	-35.865	-46.138	8.403
1300	8.931	68.834	62.157	8.680	-36.372	-46.972	7.897
1400	8.950	69.497	62.658	9.575	-36.879	-47.770	7.457
1500	8.967	70.115	63.135	10.470	-37.389	-48.530	7.071
1600	8.985	70.694	63.589	11.368	-37.899	-49.255	6.728
1700	9.003	71.239	64.023	12.267	-38.411	-49.949	6.421
1800	9.025	71.754	64.438	13.169	-38.923	-50.612	6.145
1900	9.052	72.243	64.836	14.073	-39.436	-51.247	5.895
2000	9.086	72.708	65.218	14.979	-39.950	-51.857	5.667

Phase changes: 582 K, α - β transition point of Ba; $\Delta H° = 0$ kcal/mol.
768 K, β - γ transition point of Ba; $\Delta H° = 0$ kcal/mol.
1002 K, melting point of Ba; $\Delta H° = 1.852$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.680 + 0.222\times10^{-3}T - 0.785\times10^{5}T^{-2}$

$H°- H°_{298} = 8.680\times10^{-3}T + 0.111\times10^{-6}T^{2} + 0.785\times10^{2}T^{-1} - 2.861$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = -34.217 + 14.788\times10^{-3}T - 18.390\times10^{-6}T^{2} + 549.400T^{-1}$

$\Delta Gf° = -34.217 - 14.788\times10^{-3}T\ln T + 18.390\times10^{-6}T^{2} + 274.700T^{-1} + 74.340\times10^{-3}T$

582-768 K: $\Delta Hf° = -30.696 + 2.548\times10^{-3}T - 5.250\times10^{-6}T^{2} + 55.900T^{-1}$

$\Delta Gf° = -30.696 - 2.548\times10^{-3}T\ln T + 5.250\times10^{-6}T^{2} + 27.950T^{-1} - 1.260\times10^{-3}T$

768-1002 K: $\Delta Hf° = -27.740 - 5.594\times10^{-3}T + 0.340\times10^{-6}T^{2} + 55.500T^{-1}$

$\Delta Gf° = -27.740 + 5.594\times10^{-3}T\ln T - 0.340\times10^{-6}T^{2} + 27.750T^{-1} - 54.908\times10^{-3}T$

1002-2000 K: $\Delta Hf° = -34.994 - 1.527\times10^{-3}T - 0.789\times10^{-6}T^{2} + 2521.800T^{-1}$

$\Delta Gf° = -34.994 + 1.527\times10^{-3}T\ln T + 0.789\times10^{-6}T^{2} + 1260.900T^{-1} - 21.927\times10^{-3}T$

Source: Data from Chase (33).

Be(c,l)

Beryllium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	3.930	2.270	2.270	0
300	3.950	2.290	2.270	.007
400	4.720	3.540	2.433	.443
500	5.260	4.650	2.762	.944
600	5.610	5.650	3.168	1.489
700	5.880	6.530	3.581	2.064
800	6.080	7.330	4.003	2.662
900	6.280	8.060	4.417	3.279
1000	6.500	8.730	4.813	3.917
1100	6.720	9.360	5.197	4.579
1200	6.950	9.950	5.565	5.262
1300	7.170	10.520	5.929	5.968
1400	7.380	11.060	6.277	6.696
1500	7.580	11.570	6.607	7.445
1527	7.610	11.710	6.700	7.651
1527*	7.700	12.110	6.700	8.262
1560	7.700	12.270	6.811	8.516
1560	7.040	14.140	6.811	11.435
1600	7.040	14.320	6.997	11.717
1700	7.040	14.740	7.434	12.421
1800	7.040	15.140	7.848	13.125
1900	7.040	15.530	8.252	13.829
2000	7.040	15.890	8.624	14.533
2100	7.040	16.230	8.974	15.237
2200	7.040	16.560	9.314	15.941
2300	7.040	16.870	9.633	16.645
2400	7.040	17.170	9.941	17.349
2500	7.040	17.460	10.239	18.053

*Enthalpies of transition and fusion, and data for Be(β) estimated. Data above 2200 K extrapolated.

Phase changes: 1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.
2745 K, boiling point of Be; ΔH° = 69.9 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1527 K: $Cp^\circ = 4.741 + 1.924\times10^{-3}T - 1.231\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.741\times10^{-3}T + 0.962\times10^{-6}T^2 + 1.231\times10^{2}T^{-1} - 1.912$

1527-1560 K: $Cp^\circ = 7.700$

$H^\circ - H^\circ_{298} = 7.700\times10^{-3}T - 3.496$

1560-2500 K: $Cp^\circ = 7.040$

$H^\circ - H^\circ_{298} = 7.040\times10^{-3}T + 0.453$

Source: Data from Hultgren (99) who estimated entropies of transition and fusion and extrapolated above 2200 K by assuming constant heat capacity.

Be(g)

Beryllium (ideal monatomic gas)

[Formation: Be(c,l) = Be(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^{\circ}_{298})/T$	$H°- H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	4.968	32.545	32.545	0	77.400	68.374	-50.118
300	4.968	32.576	32.546	.009	77.402	68.316	-49.768
400	4.968	34.005	32.740	.506	77.463	65.277	-35.665
500	4.968	35.114	33.108	1.003	77.459	62.227	-27.199
600	4.968	36.019	33.519	1.500	77.411	59.190	-21.560
700	4.968	36.785	33.934	1.996	77.332	56.154	-17.532
800	4.968	37.449	34.333	2.493	77.231	53.136	-14.516
900	4.968	38.034	34.712	2.990	77.111	50.134	-12.174
1000	4.968	38.557	35.070	3.487	76.970	47.143	-10.303
1100	4.968	39.031	35.409	3.984	76.805	44.167	-8.775
1200	4.968	39.463	35.729	4.481	76.619	41.203	-7.504
1300	4.968	39.861	36.033	4.977	76.409	38.266	-6.433
1400	4.968	40.229	36.319	5.474	76.178	35.341	-5.517
1500	4.968	40.572	36.591	5.971	75.926	32.423	-4.724
1527	4.968	40.661	36.663	6.105	75.854	31.647	-4.529
1527	4.968	40.661	36.663	6.105	75.243	31.647	-4.529
1560	4.968	40.766	36.747	6.269	75.153	30.698	-4.301
1560	4.968	40.766	36.747	6.269	72.234	30.698	-4.301
1600	4.968	40.892	36.849	6.468	72.151	29.636	-4.048
1700	4.968	41.193	37.096	6.965	71.944	26.974	-3.468
1800	4.968	41.477	37.332	7.461	71.736	24.329	-2.954
1900	4.968	41.746	37.558	7.958	71.529	21.719	-2.498
2000	4.969	42.001	37.773	8.455	71.322	19.100	-2.087

Phase changes: 1527 K, α - β transition point of Be; $\Delta H° = 0.611$ kcal/mol.
1560 K, melting point of Be; $\Delta H° = 2.919$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.968$

$H°- H^{\circ}_{298} = 4.968\times10^{-3}T - 1.481$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = 77.831 + 0.227\times10^{-3}T - 0.962\times10^{-6}T^2 - 123.100T^{-1}$

$\Delta Gf° = 77.831 - 0.227\times10^{-3}T\ln T + 0.962\times10^{-6}T^2 - 61.550T^{-1} - 30.021\times10^{-3}T$

1527-1560 K: $\Delta Hf° = 79.414 - 2.732\times10^{-3}T$

$\Delta Gf° = 79.414 + 2.732\times10^{-3}T\ln T - 51.308\times10^{-3}T$

1560-2000 K: $\Delta Hf° = 75.466 - 2.072\times10^{-3}T$

$\Delta Gf° = 75.466 + 2.072\times10^{-3}T\ln T - 43.924\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (36). All other data from JANAF (51).

BeO(c)

Beryllium Oxide

[Formation: $Be(c,l) + 0.5O_2(g) = BeO(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	6.110	3.290	3.290	0	-145.600	-138.599	101.594
300	6.153	3.328	3.291	.011	-145.603	-138.557	100.937
400	8.033	5.378	3.555	.729	-145.676	-136.193	74.411
500	9.279	7.313	4.117	1.598	-145.673	-133.824	58.494
600	10.148	9.087	4.800	2.572	-145.622	-131.455	47.882
700	10.757	10.699	5.529	3.619	-145.538	-129.103	40.307
800	11.185	12.165	6.269	4.717	-145.438	-126.762	34.629
900	11.489	13.501	6.999	5.852	-145.327	-124.430	30.215
1000	11.711	14.724	7.712	7.012	-145.218	-122.117	26.688
1100	11.885	15.849	8.402	8.192	-145.120	-119.813	23.804
1200	12.036	16.889	9.065	9.389	-145.030	-117.520	21.403
1300	12.183	17.858	9.704	10.600	-144.952	-115.223	19.371
1400	12.335	18.767	10.321	11.825	-144.888	-112.940	17.631
1500	12.502	19.623	10.912	13.067	-144.829	-110.669	16.124
1527	12.552	19.846	11.068	13.405	-144.815	-110.049	15.750
1527	12.552	19.846	11.068	13.405	-145.426	-110.049	15.750
1560	12.612	20.116	11.257	13.820	-145.410	-109.293	15.311
1560	12.612	20.116	11.257	13.820	-148.329	-109.293	15.311
1600	12.686	20.436	11.482	14.326	-148.281	-108.291	14.792
1700	12.885	21.211	12.032	15.605	-148.147	-105.807	13.602
1800	13.097	21.954	12.563	16.904	-147.996	-103.325	12.545
1900	13.317	22.667	13.075	18.225	-147.826	-100.829	11.598
2000	13.537	23.356	13.573	19.567	-147.638	-98.364	10.749
2100	13.752	24.022	14.054	20.932	-147.429	-95.912	9.982
2200	13.954	24.666	14.522	22.317	-147.203	-93.458	9.284
2300	14.138	25.291	14.977	23.722	-146.960	-91.029	8.650
2373	14.260	25.734	15.301	24.758	-146.774	-89.255	8.220
2373*	16.000	26.303	15.301	26.108	-145.424	-89.255	8.220
2400	16.000	26.484	15.426	26.540	-145.307	-88.616	8.069
2500	16.000	27.137	15.881	28.140	-144.874	-86.256	7.540

*Data for BeO(β) estimated.

Phase changes: 1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.
2373 K, α - β transition point of BeO; ΔH° = 1.350 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2373 K: $Cp° = 10.239 + 1.704\times10^{-3}T - 4.121\times10^{5}T^{-2}$

$H°- H°_{298} = 10.239\times10^{-3}T + 0.852\times10^{-6}T^{2} + 4.121\times10^{2}T^{-1} - 4.511$

2373-2500 K: $Cp° = 16.000$

$H°- H°_{298} = 16.000\times10^{-3}T - 11.860$

BeO(c) - Continued

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf^\circ = -147.023 + 1.883\times10^{-3}T - 0.361\times10^{-6}T^2 + 266.400T^{-1}$

$\Delta Gf^\circ = -147.023 - 1.883\times10^{-3}T\ln T + 0.361\times10^{-6}T^2 + 133.200T^{-1} + 37.377\times10^{-3}T$

1527-1560 K: $\Delta Hf^\circ = -145.439 - 1.076\times10^{-3}T + 0.601\times10^{-6}T^2 + 389.500T^{-1}$

$\Delta Gf^\circ = -145.439 + 1.076\times10^{-3}T\ln T - 0.601\times10^{-6}T^2 + 194.750T^{-1} + 16.090\times10^{-3}T$

1560-2000 K: $\Delta Hf^\circ = -149.388 - 0.416\times10^{-3}T + 0.601\times10^{-6}T^2 + 389.500T^{-1}$

$\Delta Gf^\circ = -149.388 + 0.416\times10^{-3}T\ln T - 0.601\times10^{-6}T^2 + 194.750T^{-1} + 23.474\times10^{-3}T$

2000-2373 K: $\Delta Hf^\circ = -148.720 - 0.971\times10^{-3}T + 0.748\times10^{-6}T^2 + 97.100T^{-1}$

$\Delta Gf^\circ = -148.720 + 0.971\times10^{-3}T\ln T - 0.748\times10^{-6}T^2 + 48.550T^{-1} + 19.252\times10^{-3}T$

2373-2500 K: $\Delta Hf^\circ = -156.069 + 4.790\times10^{-3}T - 0.105\times10^{-6}T^2 - 315.000T^{-1}$

$\Delta Gf^\circ = -156.069 - 4.790\times10^{-3}T\ln T + 0.105\times10^{-6}T^2 - 157.500T^{-1} + 65.137\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (36). Low-temperature heat capacities from Furukawa (71). High-temperature data based on Victor (235), Rodigina (188), and Kandyba (113). Enthalpy and temperature of transition from Conway (40). Heat capacity for BeO(β) estimated.

BeO(g)

Beryllium Oxide (ideal gas)

[Formation: $Be(c,l) + 0.5O_2(g) = BeO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.046	47.207	47.207	0	32.600	26.507	-19.430
300	7.049	47.250	47.207	.013	32.599	26.469	-19.282
400	7.253	49.304	47.486	.727	32.522	24.435	-13.350
500	7.510	50.950	48.020	1.465	32.394	22.424	-9.802
600	7.757	52.341	48.626	2.229	32.236	20.450	-7.449
700	7.969	53.553	49.244	3.016	32.058	18.496	-5.775
800	8.146	54.629	49.852	3.822	31.867	16.572	-4.527
900	8.294	55.598	50.438	4.644	31.665	14.675	-3.563
1000	8.425	56.478	50.998	5.480	31.450	12.797	-2.797
1100	8.552	57.287	51.533	6.329	31.217	10.942	-2.174
1200	8.689	58.037	52.044	7.191	30.972	9.105	-1.658
1300	8.849	58.739	52.534	8.067	30.715	7.298	-1.227
1400	9.040	59.401	53.000	8.962	30.450	5.509	-.860
1500	9.270	60.033	53.448	9.877	30.180	3.726	-.543
1527	9.344	60.199	53.566	10.128	30.108	3.256	-.466
1527	9.344	60.199	53.566	10.128	29.497	3.256	-.466
1560	9.434	60.399	53.708	10.437	29.407	2.683	-.376
1560	9.434	60.399	53.708	10.437	26.488	2.683	-.376
1600	9.543	60.639	53.878	10.817	26.410	2.075	-.283
1700	9.855	61.227	54.293	11.787	26.235	.548	-.070
1800	10.205	61.800	54.695	12.789	26.089	-.963	.117
1900	10.584	62.362	55.084	13.829	25.978	-2.445	.281
2000	10.984	62.915	55.462	14.907	25.903	-3.942	.431

Phase changes: 1527 K, α − β transition point of Be; $\Delta H° = 0.611$ kcal/mol.
1560 K, melting point of Be; $\Delta H° = 2.919$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.617 + 1.852\times10^{-3}T - 0.109\times10^{5}T^{-2}$

$H°- H°_{298} = 6.617\times10^{-3}T + 0.926\times10^{-6}T^{2} + 0.109\times10^{2}T^{-1} - 2.092$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = 33.596 - 1.739\times10^{-3}T - 0.287\times10^{-6}T^{2} - 134.800T^{-1}$

$\Delta Gf° = 33.596 + 1.739\times10^{-3}T\ln T + 0.287\times10^{-6}T^{2} - 67.400T^{-1} - 33.011\times10^{-3}T$

1527-1560 K: $\Delta Hf° = 35.180 - 4.698\times10^{-3}T + 0.675\times10^{-6}T^{2} - 11.700T^{-1}$

$\Delta Gf° = 35.180 + 4.698\times10^{-3}T\ln T - 0.675\times10^{-6}T^{2} - 5.850T^{-1} - 54.298\times10^{-3}T$

1560-2000 K: $\Delta Hf° = 31.231 - 4.038\times10^{-3}T + 0.675\times10^{-6}T^{2} - 11.700T^{-1}$

$\Delta Gf° = 31.231 + 4.038\times10^{-3}T\ln T - 0.675\times10^{-6}T^{2} - 5.850T^{-1} - 46.915\times10^{-3}T$

Source: Data from Chase (32).

$(BeO)_2(g)$

Dimeric Beryllium Oxide (ideal gas)

[Formation: $2Be(c,l) + O_2(g) = (BeO)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.792	59.156	59.156	0	-103.000	-104.673	76.726
300	11.831	59.229	59.156	.022	-103.005	-104.685	76.262
400	13.689	62.897	59.642	1.302	-103.307	-105.198	57.477
500	15.105	66.112	60.622	2.745	-103.597	-105.642	46.176
600	16.146	68.963	61.780	4.310	-103.877	-106.017	38.616
700	16.911	71.512	62.991	5.965	-104.150	-106.359	33.206
800	17.477	73.809	64.201	7.686	-104.423	-106.654	29.136
900	17.904	75.893	65.386	9.456	-104.701	-106.910	25.961
1000	18.231	77.797	66.534	11.263	-104.997	-107.144	23.416
1100	18.486	79.547	67.639	13.099	-105.324	-107.345	21.327
1200	18.687	81.165	68.700	14.958	-105.679	-107.523	19.582
1300	18.849	82.667	69.716	16.836	-106.069	-107.647	18.097
1400	18.980	84.069	70.693	18.727	-106.498	-107.752	16.821
1500	19.088	85.382	71.628	20.631	-106.962	-107.846	15.713
1527	19.112	85.723	71.874	21.147	-107.094	-107.848	15.435
1527	19.112	85.723	71.874	21.147	-108.316	-107.848	15.435
1560	19.142	86.132	72.172	21.778	-108.483	-107.854	15.110
1560	19.142	86.132	72.172	21.778	-114.321	-107.854	15.110
1600	19.178	86.617	72.527	22.544	-114.470	-107.683	14.709
1700	19.254	87.782	73.390	24.466	-114.838	-107.270	13.790
1800	19.318	88.885	74.221	26.395	-115.205	-106.822	12.970
1900	19.372	89.930	75.020	28.329	-115.573	-106.310	12.228
2000	19.419	90.925	75.791	30.269	-115.940	-105.818	11.563

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1527 K, α - β transition point of Be; $\Delta H° = 0.611$ kcal/mol.
1560 K, melting point of Be; $\Delta H° = 2.919$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 15.875 + 2.378\times10^{-3}T - 4.259\times10^{5}T^{-2}$

$H°- H°_{298} = 15.875\times10^{-3}T + 1.189\times10^{-6}T^2 + 4.259\times10^{2}T^{-1} - 6.267$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = -103.092 - 0.837\times10^{-3}T - 1.238\times10^{-6}T^2 + 134.500T^{-1}$

$\Delta Gf° = -103.092 + 0.837\times10^{-3}T\ln T + 1.238\times10^{-6}T^2 + 67.250T^{-1} - 11.199\times10^{-3}T$

1527-1560 K: $\Delta Hf° = -99.924 - 6.755\times10^{-3}T + 0.686\times10^{-6}T^2 + 380.700T^{-1}$

$\Delta Gf° = -99.924 + 6.755\times10^{-3}T\ln T - 0.686\times10^{-6}T^2 + 190.350T^{-1} - 53.773\times10^{-3}T$

1560-2000 K: $\Delta Hf° = -107.821 - 5.435\times10^{-3}T + 0.686\times10^{-6}T^2 + 380.700T^{-1}$

$\Delta Gf° = -107.821 + 5.435\times10^{-3}T\ln T - 0.686\times10^{-6}T^2 + 190.350T^{-1} - 39.005\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (180). All other data are those estimated by JANAF (51).

$(BeO)_4(g)$

Tetrameric Beryllium Oxide (ideal gas)

[Formation: $4Be(c,l) + 2O_2(g) = (BeO)_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	21.364	72.292	72.292	0	-391.000	-380.625	279.002
300	21.473	72.425	72.292	.040	-391.014	-380.564	277.237
400	26.784	79.358	73.201	2.463	-391.755	-376.962	205.960
500	30.818	85.792	75.086	5.353	-392.331	-373.206	163.126
600	33.745	91.684	77.369	8.589	-392.785	-369.319	134.523
700	35.860	97.053	79.803	12.075	-393.155	-365.394	114.080
800	37.407	101.948	82.271	15.742	-393.476	-361.402	98.729
900	38.559	106.423	84.709	19.543	-393.771	-357.361	86.778
1000	39.434	110.533	87.088	23.445	-394.075	-353.308	77.214
1100	40.110	114.325	89.394	27.424	-394.422	-349.217	69.382
1200	40.642	117.838	91.620	31.462	-394.812	-345.110	62.852
1300	41.067	121.109	93.764	35.549	-395.261	-340.925	57.314
1400	41.412	124.165	95.827	39.673	-395.777	-336.724	52.564
1500	41.694	127.033	97.814	43.829	-396.357	-332.527	48.449
1527	41.757	127.777	98.337	44.956	-396.526	-331.354	47.424
1527	41.757	127.777	98.337	44.956	-398.970	-331.354	47.424
1560	41.835	128.671	98.969	46.335	-399.187	-329.924	46.220
1560	41.835	128.671	98.969	46.335	-410.863	-329.924	46.220
1600	41.929	129.731	99.725	48.010	-411.018	-327.839	44.780
1700	42.125	132.279	101.565	52.213	-411.395	-322.674	41.482
1800	42.291	134.692	103.340	56.434	-411.766	-317.460	38.544
1900	42.433	136.982	105.050	60.671	-412.133	-312.140	35.904
2000	42.555	139.162	106.702	64.920	-412.498	-306.878	33.534

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1527 K, α - β transition point of Be; $\Delta H°$ = 0.611 kcal/mol.
1560 K, melting point of Be; $\Delta H°$ = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 33.285 + 6.268\times10^{-3}T - 12.258\times10^{5}T^{-2}$

$H°- H°_{298} = 33.285\times10^{-3}T + 3.134\times10^{-6}T^{2} + 12.258\times10^{2}T^{-1} - 14.314$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = -392.962 - 0.139\times10^{-3}T - 1.720\times10^{-6}T^{2} + 643.000T^{-1}$

$\Delta Gf° = -392.962 + 0.139\times10^{-3}T\ln T + 1.720\times10^{-6}T^{2} + 321.500T^{-1} + 36.458\times10^{-3}T$

1527-1560 K: $\Delta Hf° = -386.628 - 11.975\times10^{-3}T + 2.128\times10^{-6}T^{2} + 1135.400T^{-1}$

$\Delta Gf° = -386.628 + 11.975\times10^{-3}T\ln T - 2.128\times10^{-6}T^{2} + 567.700T^{-1} - 48.690\times10^{-3}T$

1560-2000 K: $\Delta Hf° = -402.422 - 9.335\times10^{-3}T + 2.128\times10^{-6}T^{2} + 1135.400T^{-1}$

$\Delta Gf° = -402.422 + 9.335\times10^{-3}T\ln T - 2.128\times10^{-6}T^{2} + 567.700T^{-1} - 19.155\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (180). All other data are those estimated by JANAF (51).

$(BeO)_6(g)$

Hexameric Boron Oxide (ideal gas)

[Formation: $6Be(c,l) + 3O_2(g) = (BeO)_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	31.459	82.000	82.000	0	-651.000	-627.555	460.004
300	31.644	82.195	82.002	.058	-651.023	-627.415	457.066
400	40.551	92.573	83.355	3.687	-652.140	-619.365	338.401
500	47.149	102.371	86.189	8.091	-652.935	-611.089	267.103
600	51.861	111.408	89.651	13.054	-653.507	-602.637	219.508
700	55.231	119.670	93.359	18.418	-653.927	-594.148	185.499
800	57.682	127.214	97.126	24.070	-654.257	-585.580	159.971
900	59.499	134.117	100.858	29.933	-654.538	-576.958	140.103
1000	60.874	140.461	104.506	35.955	-654.825	-568.336	124.208
1100	61.935	146.315	108.044	42.098	-655.171	-559.674	111.196
1200	62.769	151.741	111.462	48.335	-655.576	-551.004	100.350
1300	63.434	156.792	114.757	54.646	-656.069	-542.232	91.156
1400	63.972	161.513	117.929	61.017	-656.658	-533.450	83.274
1500	64.413	165.943	120.985	67.437	-657.342	-524.688	76.446
1527	64.512	167.093	121.790	69.177	-657.546	-522.264	74.747
1527	64.512	167.093	121.790	69.177	-661.212	-522.264	74.747
1560	64.632	168.474	122.763	71.309	-661.473	-519.306	72.752
1560	64.632	168.474	122.763	71.309	-678.987	-519.306	72.752
1600	64.778	170.112	123.926	73.897	-679.145	-515.201	70.372
1700	65.085	174.048	126.759	80.391	-679.521	-505.009	64.923
1800	65.344	177.776	129.491	86.913	-679.887	-494.757	60.071
1900	65.565	181.315	132.127	93.458	-680.248	-484.358	55.713
2000	65.754	184.683	134.671	100.024	-680.603	-474.053	51.801

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1527 K, α - β transition point of Be; $\Delta H° = 0.611$ kcal/mol.
1560 K, melting point of Be; $\Delta H° = 2.919$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 51.598 + 9.612\times10^{-3}T - 20.449\times10^{5}T^{-2}$

$H°- H°_{298} = 51.598\times10^{-3}T + 4.806\times10^{-6}T^{2} + 20.449\times10^{2}T^{-1} - 22.670$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = -655.142 + 1.462\times10^{-3}T - 2.475\times10^{-6}T^{2} + 1170.700T^{-1}$

$\Delta Gf° = -655.142 - 1.462\times10^{-3}T\ln T + 2.475\times10^{-6}T^{2} + 585.350T^{-1} + 93.536\times10^{-3}T$

1527-1560 K: $\Delta Hf° = -645.641 - 16.292\times10^{-3}T + 3.297\times10^{-6}T^{2} + 1909.300T^{-1}$

$\Delta Gf° = -645.641 + 16.292\times10^{-3}T\ln T - 3.297\times10^{-6}T^{2} + 954.650T^{-1} - 34.187\times10^{-3}T$

1560-2000 K: $\Delta Hf° = -669.332 - 12.332\times10^{-3}T + 3.297\times10^{-6}T^{2} + 1909.300T^{-1}$

$\Delta Gf° = -669.332 + 12.332\times10^{-3}T\ln T - 3.297\times10^{-6}T^{2} + 954.650T^{-1} + 10.116\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (180). All other data are those estimated by JANAF (51).

Bi(c,1)

Bismuth

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.100	13.560	13.560	0
300	6.100	13.600	13.563	.011
400	6.350	15.380	13.800	.632
500	6.850	16.850	14.270	1.290
544.59	7.140	17.440	14.500	1.601
544.59	7.300	22.400	14.500	4.301
600	7.040	23.090	15.260	4.698
700	6.850	24.160	16.459	5.391
800	6.720	25.070	17.484	6.069
900*	6.620	25.850	18.366	6.736
1000	6.550	26.550	19.155	7.395
1100	6.510	27.170	19.854	8.048
1200	6.500	27.740	20.492	8.698
1300	6.500	28.260	21.069	9.348
1400	6.500	28.740	21.599	9.998
1500	6.500	29.190	22.091	10.648
1600	6.500	29.610	22.549	11.298
1700	6.500	30.000	22.972	11.948
1800	6.500	30.370	23.371	12.598
1837	6.500	30.500	23.511	12.838

*Data above 800 K extrapolated.

Phase changes: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.
1837 K, boiling point of Bi to equilibrium mixture of Bi(g) and Bi_2(g).

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-544.59 K: $Cp^\circ = 3.323 + 6.404\times10^{-3}T + 0.771\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 3.323\times10^{-3}T + 3.202\times10^{-6}T^2 - 0.771\times10^{2}T^{-1} - 1.017$

544.59-1837 K: $Cp^\circ = 5.853 + 0.318\times10^{-3}T + 3.777\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.853\times10^{-3}T + 0.159\times10^{-6}T^2 - 3.777\times10^{2}T^{-1} + 1.760$

Source: Data from Hultgren (99) who extrapolated above 800 K.

Bi(g)

Bismuth (ideal monatomic gas)

[Formation: Bi(c,l) = Bi(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	44.669	44.669	0	49.500	40.225	-29.485
300	4.968	44.700	44.670	.009	49.498	40.168	-29.262
400	4.968	46.129	44.864	.506	49.374	37.074	-20.256
500	4.968	47.238	45.232	1.003	49.213	34.019	-14.870
544.59	4.968	47.662	45.414	1.225	49.124	32.666	-13.109
544.59	4.968	47.662	45.414	1.225	46.424	32.666	-13.109
600	4.968	48.144	45.644	1.500	46.302	31.270	-11.390
700	4.968	48.910	46.059	1.996	46.105	28.780	-8.985
800	4.968	49.573	46.457	2.493	45.924	26.322	-7.191
900	4.968	50.158	46.836	2.990	45.754	23.877	-5.798
1000	4.968	50.682	47.195	3.487	45.592	21.460	-4.690
1100	4.968	51.155	47.533	3.984	45.436	19.053	-3.785
1200	4.968	51.587	47.854	4.480	45.282	16.666	-3.035
1300	4.969	51.985	48.157	4.977	45.129	14.287	-2.402
1400	4.970	52.353	48.443	5.474	44.976	11.918	-1.860
1500	4.972	52.696	48.715	5.971	44.823	9.564	-1.393
1600	4.976	53.017	48.974	6.469	44.671	7.220	-.986
1700	4.981	53.319	49.221	6.966	44.518	4.876	-.627
1800	4.988	53.604	49.457	7.465	44.367	2.546	-.309

Phase change: 544.59 K, melting point of Bi; $\Delta H° = 2.700$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 4.961 + 0.008\times10^{-3}T + 0.004\times10^{5}T^{-2}$

$H°- H°_{298} = 4.961\times10^{-3}T + 0.004\times10^{-6}T^{2} - 0.004\times10^{2}T^{-1} - 1.478$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf° = 49.039 + 1.638\times10^{-3}T - 3.198\times10^{-6}T^{2} + 76.700T^{-1}$

$\Delta Gf° = 49.039 - 1.638\times10^{-3}T\ln T + 3.198\times10^{-6}T^{2} + 38.350T^{-1} - 21.614\times10^{-3}T$

544.59-1800 K: $\Delta Hf° = 46.262 - 0.892\times10^{-3}T - 0.155\times10^{-6}T^{2} + 377.300T^{-1}$

$\Delta Gf° = 46.262 + 0.892\times10^{-3}T\ln T + 0.155\times10^{-6}T^{2} + 188.650T^{-1} - 31.304\times10^{-3}T$

Sources: Enthalpy of formation at 298 from Wagman (236). All other data from Hilsenrath (94).

$Bi_2(g)$

Bismuth (ideal diatomic gas)

[Formation: $2Bi(c,l) = Bi_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.830	65.400	65.400	0	52.600	41.187	-30.190
300	8.831	65.455	65.402	.016	52.594	41.117	-29.954
400	8.880	68.002	65.747	.902	52.238	37.341	-20.402
500	8.900	69.986	66.406	1.790	51.810	33.667	-14.716
544.59	8.904	70.746	66.731	2.187	51.585	32.054	-12.864
544.59	8.904	70.746	66.731	2.187	46.185	32.054	-12.864
600	8.910	71.610	67.140	2.682	45.886	30.628	-11.156
700	8.920	72.984	67.881	3.572	45.390	28.125	-8.781
800	8.930	74.176	68.594	4.466	44.928	25.699	-7.021
900	8.930	75.226	69.273	5.358	44.486	23.313	-5.661
1000	8.930	76.168	69.916	6.252	44.062	20.994	-4.588
1100	8.930	77.018	70.523	7.144	43.648	18.702	-3.716
1200	8.940	77.796	71.098	8.038	43.242	16.463	-2.998
1300	8.940	78.512	71.641	8.932	42.836	14.246	-2.395
1400	8.940	79.174	72.155	9.826	42.430	12.058	-1.882
1500	8.940	79.792	72.645	10.720	42.024	9.906	-1.443
1600	8.940	80.368	73.109	11.614	41.618	7.781	-1.063
1700	8.940	80.910	73.552	12.508	41.212	5.665	-.728
1800	8.940	81.422	73.976	13.402	40.806	3.578	-.434

Phase change: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol of Bi.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp^\circ = 8.942 - 0.099\times10^5T^{-2}$

$H^\circ - H^\circ_{298} = 8.942\times10^{-3}T + 0.099\times10^2T^{-1} - 2.699$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf^\circ = 51.934 + 2.296\times10^{-3}T - 6.404\times10^{-6}T^2 + 164.100T^{-1}$

$\Delta Gf^\circ = 51.934 - 2.296\times10^{-3}T\ln T + 6.404\times10^{-6}T^2 + 82.050T^{-1} - 25.798\times10^{-3}T$

544.59-1800 K: $\Delta Hf^\circ = 46.381 - 2.764\times10^{-3}T - 0.318\times10^{-6}T^2 + 765.300T^{-1}$

$\Delta Gf^\circ = 46.381 + 2.764\times10^{-3}T\ln T + 0.318\times10^{-6}T^2 + 382.650T^{-1} - 45.178\times10^{-3}T$

Source: Data from Hultgren (99).

Bi_2O_3(c,1)

Dibismuth Trioxide

[Formation: $2Bi(c,1) + 1.5O_2(g) = Bi_2O_3(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	27.130	36.200	36.200	0	-137.160	-117.951	86.459
300	27.174	36.368	36.201	.050	-137.152	-117.830	85.838
400	28.705	44.419	37.286	2.853	-136.656	-111.465	60.901
500	29.524	50.920	39.386	5.767	-136.154	-105.223	45.992
544.59	29.780	53.453	40.436	7.089	-135.954	-102.478	41.125
544.59	29.780	53.453	40.436	7.089	-141.354	-102.478	41.125
600	30.097	56.356	41.773	8.750	-141.120	-98.538	35.892
700	30.595	61.033	44.199	11.784	-140.639	-91.477	28.560
800	31.090	65.150	46.564	14.869	-140.107	-84.483	23.079
900	31.616	68.842	48.838	18.004	-139.527	-77.574	18.837
1000	32.191	72.203	51.010	21.193	-138.896	-70.714	15.454
1003	32.209	72.299	51.073	21.290	-138.876	-70.509	15.363
1003	33.100	79.816	51.072	28.830	-131.336	-70.509	15.363
1098	33.100	82.812	53.691	31.975	-130.627	-64.784	12.895
1098	43.000	86.455	53.691	35.975	-126.627	-64.784	12.895
1100	43.000	86.533	53.750	36.061	-126.593	-64.671	12.849
1200	43.000	90.275	56.641	40.361	-124.865	-59.108	10.765
1300	43.000	93.717	59.362	44.661	-123.149	-53.699	9.028

Phase changes: 544.59 K, melting point of Bi; $\Delta H°$ = 2.700 kcal/mol.
1003 K, α - δ transition point of Bi_2O_3; $\Delta H°$ = 7.540 kcal/mol.
1098 K, melting point of Bi_2O_3; $\Delta H°$ = 4.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1003 K:
$$Cp° = 28.586 + 3.652\times10^{-3}T - 2.262\times10^{5}T^{-2}$$
$$H°- H°_{298} = 28.586\times10^{-3}T + 1.826\times10^{-6}T^{2} + 2.262\times10^{2}T^{-1} - 9.444$$

1003-1098 K:
$$Cp° = 33.100$$
$$H°- H°_{298} = 33.100\times10^{-3}T - 4.369$$

1098-1300 K:
$$Cp° = 43.000$$
$$H°- H°_{298} = 43.000\times10^{-3}T - 11.239$$

Formation equations (kcal/mol):

298.15-544.59 K:
$$\Delta Hf° = -141.042 + 11.095\times10^{-3}T - 5.333\times10^{-6}T^{2} + 312.600T^{-1}$$
$$\Delta Gf° = -141.042 - 11.095\times10^{-3}T\ln T + 5.333\times10^{-6}T^{2} + 156.300T^{-1} + 137.316\times10^{-3}T$$

544.59-1003 K:
$$\Delta Hf° = -146.596 + 6.035\times10^{-3}T + 0.753\times10^{-6}T^{2} + 913.800T^{-1}$$
$$\Delta Gf° = -146.596 - 6.035\times10^{-3}T\ln T - 0.753\times10^{-6}T^{2} + 456.900T^{-1} + 117.936\times10^{-3}T$$

1003-1098 K:
$$\Delta Hf° = -141.521 + 10.549\times10^{-3}T - 1.072\times10^{-6}T^{2} + 687.600T^{-1}$$
$$\Delta Gf° = -141.521 - 10.549\times10^{-3}T\ln T + 1.072\times10^{-6}T^{2} + 343.800T^{-1} + 142.352\times10^{-3}T$$

1098-1300 K:
$$\Delta Hf° = -148.391 + 20.449\times10^{-3}T - 1.072\times10^{-6}T^{2} + 687.600T^{-1}$$
$$\Delta Gf° = -148.391 - 20.449\times10^{-3}T\ln T + 1.072\times10^{-6}T^{2} + 343.800T^{-1} + 217.921\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities and entropy at 298 K from Anderson (3). High-temperature data based on Cubicciotti (47). Temperature of fusion from Levin (144) whose enthalpy of fusion agrees with Cubicciotti.

$Br_2(l,g)$

Bromine

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	18.090	36.379	36.379	0
300	18.077	36.491	36.381	.033
332.6	18.028	38.350	36.483	.621
332.6	8.683	59.592	36.483	7.686
400	8.775	61.197	40.509	8.275
500	8.857	63.164	44.850	9.157
600	8.908	64.784	48.042	10.045
700	8.944	66.160	50.534	10.938
800	8.970	67.356	52.565	11.833
900	8.992	68.414	54.267	12.732
1000	9.011	69.362	55.730	13.632
1100	9.027	70.222	57.009	14.534
1200	9.042	71.008	58.144	15.437
1300	9.056	71.732	59.161	16.342
1400	9.069	72.404	60.084	17.248
1500	9.082	73.030	60.926	18.156
1600	9.094	73.617	61.701	19.065
1700	9.106	74.168	62.418	19.975
1800	9.118	74.689	63.086	20.886
1900	9.129	75.183	63.710	21.798
2000	9.141	75.651	64.295	22.712
2100	9.152	76.097	64.847	23.626
2200	9.163	76.523	65.368	24.542
2300	9.174	76.931	65.862	25.459
2400	9.185	77.322	66.332	26.377
2500	9.196	77.697	66.779	27.296
2600	9.206	78.058	67.206	28.216
2700	9.217	78.405	67.614	29.137
2800	9.228	78.741	68.005	30.060
2900	9.238	79.065	68.381	30.983
3000	9.249	79.378	68.742	31.907

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-332.6 K:

$$Cp^\circ = 18.091 - 0.200\times10^{-3}T$$

$$H^\circ - H^\circ_{298} = 18.091\times10^{-3}T - 0.100\times10^{-6}T^2 - 5.385$$

332.6-3000 K:

$$Cp^\circ = 8.930 + 0.110\times10^{-3}T - 0.314\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 8.930\times10^{-3}T + 0.055\times10^{-6}T^2 + 0.314\times10^{2}T^{-1} + 4.615$$

Sources: Entropy of $Br_2(l)$ and enthalpy of formation of $Br_2(g)$ at 298 K from CODATA (36). All other data from JANAF (51).

Br(g)

Bromine (ideal monatomic gas)

[Formation: $0.5Br_2(l,g) = Br(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	41.803	41.803	0	26.735	19.695	-14.436
300	4.968	41.834	41.804	.009	26.728	19.651	-14.316
332.6	4.968	42.346	41.832	.171	26.595	18.889	-12.411
332.6	4.968	42.346	41.832	.171	23.063	18.889	-12.411
400	4.968	43.263	41.998	.506	23.104	18.038	-9.855
500	4.971	44.372	42.366	1.003	23.160	16.765	-7.328
600	4.979	45.279	42.779	1.500	23.213	15.480	-5.639
700	4.997	46.048	43.192	1.999	23.265	14.187	-4.429
800	5.026	46.717	43.592	2.500	23.319	12.887	-3.521
900	5.063	47.311	43.973	3.004	23.373	11.579	-2.812
1000	5.106	47.846	44.333	3.513	23.432	10.267	-2.244
1100	5.153	48.335	44.675	4.026	23.494	8.948	-1.778
1200	5.199	48.785	44.999	4.543	23.560	7.622	-1.388
1300	5.243	49.203	45.306	5.066	23.630	6.292	-1.058
1400	5.284	49.593	45.599	5.592	23.703	4.956	-.774
1500	5.320	49.959	45.878	6.122	23.779	3.613	-.526
1600	5.351	50.304	46.144	6.656	23.859	2.266	-.309
1700	5.377	50.629	46.398	7.192	23.940	.913	-.117
1800	5.398	50.937	46.642	7.731	24.023	-.443	.054
1900	5.415	51.229	46.875	8.272	24.108	-1.803	.207
2000	5.428	51.507	47.100	8.814	24.193	-3.170	.346
2100	5.437	51.772	47.316	9.357	24.279	-4.540	.473
2200	5.443	52.025	47.525	9.901	24.365	-5.915	.588
2300	5.446	52.267	47.726	10.445	24.451	-7.293	.693
2400	5.446	52.499	47.920	10.990	24.537	-8.675	.790
2500	5.445	52.721	48.107	11.535	24.622	-10.059	.879
2600	5.442	52.935	48.289	12.079	24.706	-11.450	.962
2700	5.437	53.140	48.465	12.623	24.790	-12.842	1.039
2800	5.432	53.338	48.636	13.166	24.871	-14.238	1.111
2900	5.425	53.528	48.801	13.709	24.953	-15.634	1.178
3000	5.418	53.712	48.962	14.251	25.033	-17.037	1.241

Phase change: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol of Br_2.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 4.854 + 0.264\times10^{-3}T + 0.030\times10^{5}T^{-2}$

$H°- H°_{298} = 4.854\times10^{-3}T + 0.132\times10^{-6}T^2 - 0.030\times10^{2}T^{-1} - 1.449$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = 27.979 - 4.191\times10^{-3}T + 0.182\times10^{-6}T^2 - 3.000T^{-1}$

$\Delta Gf° = 27.979 + 4.191\times10^{-3}T\ln T - 0.182\times10^{-6}T^2 - 1.500T^{-1} - 51.595\times10^{-3}T$

332.6-3000 K: $\Delta Hf° = 22.978 + 0.389\times10^{-3}T + 0.104\times10^{-6}T^2 - 18.700T^{-1}$

$\Delta Gf° = 22.978 - 0.389\times10^{-3}T\ln T - 0.104\times10^{-6}T^2 - 9.350T^{-1} - 9.917\times10^{-3}T$

Source: Data from Chase (33).

$Br_2(g)$

Bromine (ideal diatomic gas)

[Formation: $Br_2(l,g) = Br_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.616	58.640	58.640	0	7.388	0.751	-.550
300	8.620	58.693	58.640	.016	7.371	.710	-.518
332.6	8.671	59.585	58.689	.298	7.065	0	0
332.6	8.671	59.585	58.689	.298	0	0	0
400	8.775	61.197	58.979	.887	0	0	0
500	8.857	63.164	59.626	1.769	0	0	0
600	8.908	64.784	60.356	2.657	0	0	0
700	8.944	66.160	61.089	3.550	0	0	0
800	8.970	67.356	61.800	4.445	0	0	0
900	8.992	68.414	62.476	5.344	0	0	0
1000	9.011	69.362	63.118	6.244	0	0	0
1100	9.027	70.222	63.726	7.146	0	0	0
1200	9.042	71.008	64.301	8.049	0	0	0
1300	9.056	71.732	64.844	8.954	0	0	0
1400	9.069	72.404	65.361	9.860	0	0	0
1500	9.082	73.030	65.851	10.768	0	0	0
1600	9.094	73.617	66.319	11.677	0	0	0
1700	9.106	74.168	66.764	12.587	0	0	0
1800	9.118	74.689	67.190	13.498	0	0	0
1900	9.129	75.183	67.599	14.410	0	0	0
2000	9.141	75.651	67.989	15.324	0	0	0
2100	9.152	76.097	68.365	16.238	0	0	0
2200	9.163	76.523	68.726	17.154	0	0	0
2300	9.174	76.931	69.074	18.071	0	0	0
2400	9.185	77.322	69.410	18.989	0	0	0
2500	9.196	77.697	69.734	19.908	0	0	0
2600	9.206	78.058	70.047	20.828	0	0	0
2700	9.217	78.405	70.350	21.749	0	0	0
2800	9.228	78.741	70.644	22.672	0	0	0
2900	9.238	79.065	70.929	23.595	0	0	0
3000	9.249	79.378	71.205	24.519	0	0	0

Phase change: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 8.927 + 0.112\times10^{-3}T - 0.306\times10^{5}T^{-2}$

$H°- H°_{298} = 8.927\times10^{-3}T + 0.056\times10^{-6}T^2 + 0.306\times10^{2}T^{-1} - 2.769$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = 10.004 - 9.164\times10^{-3}T + 0.156\times10^{-6}T^2 + 30.600T^{-1}$

$\Delta Gf° = 10.004 + 9.164\times10^{-3}T\ln T - 0.156\times10^{-6}T^2 + 15.300T^{-1} - 83.373\times10^{-3}T$

332.6-3000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (36). All other data from JANAF (51).

C(c)

Carbon, Graphite

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	2.036	1.372	1.372	0
300	2.051	1.385	1.372	.004
400	2.824	2.083	1.463	.248
500	3.495	2.787	1.657	.565
600	4.026	3.474	1.904	.942
700	4.430	4.126	2.175	1.366
800	4.739	4.739	2.458	1.825
900	4.977	5.311	2.742	2.312
1000	5.165	5.845	3.026	2.819
1100	5.316	6.354	3.315	3.343
1200	5.441	6.813	3.579	3.881
1300	5.546	7.253	3.845	4.431
1400	5.635	7.667	4.103	4.990
1500	5.713	8.059	4.354	5.558
1600	5.782	8.430	4.598	6.132
1700	5.843	8.782	4.833	6.714
1800	5.899	9.118	5.062	7.301
1900	5.590	9.438	5.284	7.893
2000	5.997	9.745	5.499	8.491
2100	6.042	10.038	5.708	9.093
2200	6.083	10.320	5.911	9.699
2300	6.123	10.592	6.110	10.309
2400	6.160	10.853	6.301	10.924
2500	6.196	11.105	6.489	11.541
2600	6.231	11.349	6.671	12.163
2700	6.265	11.585	6.849	12.788
2800	6.297	11.813	7.022	13.416
2900	6.329	12.035	7.191	14.047
3000	6.360	12.250	7.356	14.682

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 3.518 + 1.532\times10^{-3}T - 1.723\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 3.518\times10^{-3}T + 0.766\times10^{-6}T^2 + 1.723\times10^{2}T^{-1} - 1.695$

2000-3000 K: $Cp^\circ = 5.641 + 0.268\times10^{-3}T - 7.200\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.641\times10^{-3}T + 0.134\times10^{-6}T^2 + 7.200\times10^{2}T^{-1} - 3.687$

Source: Data from JANAF (55).

C(diamond)

Carbon, Diamond

[Formation: C(graphite) = C(diamond)]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	1.462	0.566	0.566	0	0.453	0.693	-0.508
300	1.480	.576	.566	.003	.452	.695	-.506
400	2.446	1.136	.636	.200	.405	.784	-.428
500	3.242	1.771	.799	.486	.374	.882	-.386
600	3.852	2.418	1.015	.842	.353	.987	-.359
700	4.312	3.048	1.261	1.251	.338	1.093	-.341
800	4.660	3.648	1.523	1.700	.328	1.201	-.328
900	4.932	4.213	1.791	2.180	.321	1.309	-.318
1000	5.162	4.745	2.060	2.685	.319	1.419	-.310
1100	5.380	5.247	2.327	3.212	.322	1.540	-.306

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp^\circ = 1.920 + 3.646\times10^{-3}T - 1.374\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 1.920\times10^{-3}T + 1.823\times10^{-6}T^2 + 1.374\times10^{2}T^{-1} - 1.195$

Formation equations (kcal/mol):

298.15-1100 K: $\Delta Hf^\circ = 0.953 - 1.598\times10^{-3}T + 1.057\times10^{-6}T^2 - 34.900T^{-1}$

$\Delta Gf^\circ = 0.953 + 1.598\times10^{-3}T\ln T - 1.057\times10^{-6}T^2 - 17.450T^{-1} - 9.463\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from Victor (234).

C(g)

Carbon (ideal monatomic gas)

[Formation: C(c) = C(g)]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.981	37.760	37.760	0	171.290	160.441	-117.605
300	4.980	37.791	37.761	.009	171.295	160.373	-116.830
400	4.975	39.223	37.955	.507	171.549	156.693	-85.612
500	4.972	40.333	38.325	1.004	171.729	152.956	-66.856
600	4.971	41.240	38.738	1.501	171.849	149.189	-54.342
700	4.970	42.006	39.150	1.999	171.923	145.407	-45.398
800	4.970	42.669	39.550	2.495	171.960	141.616	-38.687
900	4.969	43.255	39.931	2.992	171.970	137.820	-33.467
1000	4.969	43.778	40.289	3.489	171.960	134.027	-29.291
1100	4.969	44.252	40.628	3.986	171.933	130.245	-25.877
1200	4.970	44.684	40.948	4.483	171.892	126.447	-23.029
1300	4.970	45.082	41.251	4.980	171.839	122.661	-20.621
1400	4.972	45.451	41.539	5.477	171.777	118.879	-18.558
1500	4.975	45.794	41.811	5.975	171.707	115.104	-16.770
1600	4.978	46.115	42.070	6.472	171.630	111.334	-15.207
1700	4.983	46.417	42.317	6.970	171.546	107.566	-13.828
1800	4.990	46.702	42.553	7.469	171.458	103.807	-12.604
1900	4.998	46.972	42.778	7.968	171.365	100.050	-11.508
2000	5.008	47.228	42.993	8.469	171.268	96.302	-10.523
2100	5.019	47.473	43.202	8.970	171.167	92.553	-9.632
2200	5.031	47.707	43.402	9.472	171.063	88.812	-8.823
2300	5.045	47.931	43.594	9.976	170.957	85.077	-8.084
2400	5.061	48.146	43.778	10.482	170.848	81.345	-7.407
2500	5.077	48.353	43.958	10.988	170.737	77.617	-6.785
2600	5.094	48.552	44.130	11.497	170.624	73.896	-6.211
2700	5.112	48.745	44.298	12.007	170.509	70.177	-5.680
2800	5.130	48.931	44.460	12.519	170.393	66.463	-5.188
2900	5.149	49.111	44.617	13.033	170.276	62.756	-4.729
3000	5.168	49.286	44.770	13.549	170.157	59.049	-4.302

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.952 + 0.018\times10^{-3}T + 0.021\times10^{5}T^{-2}$

$H°- H°_{298} = 4.952\times10^{-3}T + 0.009\times10^{-6}T^{2} - 0.021\times10^{2}T^{-1} - 1.470$

2000-3000 K: $Cp° = 4.419 + 0.230\times10^{-3}T + 5.160\times10^{5}T^{-2}$

$H°- H°_{298} = 4.419\times10^{-3}T + 0.115\times10^{-6}T^{2} - 5.160\times10^{2}T^{-1} - 0.571$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 171.515 + 1.434\times10^{-3}T - 0.757\times10^{-6}T^{2} - 174.400T^{-1}$

$\Delta Gf° = 171.515 - 1.434\times10^{-3}T\ln T + 0.757\times10^{-6}T^{2} - 87.200T^{-1} - 28.216\times10^{-3}T$

2000-3000 K: $\Delta Hf° = 174.405 - 1.222\times10^{-3}T - 0.019\times10^{-6}T^{2} - 1236.000T^{-1}$

$\Delta Gf° = 174.405 + 1.222\times10^{-3}T\ln T + 0.019\times10^{-6}T^{2} - 618.000T^{-1} - 48.241\times10^{-3}T$

Source: Data from JANAF (55).

$C_2(g)$

Carbon (ideal diatomic gas)

[Formation: $2C(c) = C_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	10.312	47.627	47.627	0	200.200	186.818	-136.940
300	10.301	47.690	47.627	.019	200.211	186.735	-136.035
400	9.476	50.544	48.021	1.009	200.713	182.162	-99.527
500	8.877	52.587	48.739	1.924	200.994	177.487	-77.579
600	8.604	54.178	49.520	2.795	201.111	172.773	-62.932
700	8.514	55.496	50.282	3.650	201.118	168.047	-52.466
800	8.509	56.632	51.006	4.501	201.051	163.328	-44.619
900	8.543	57.636	51.688	5.353	200.929	158.616	-38.517
1000	8.595	58.538	52.328	6.210	200.772	153.924	-33.640
1100	8.655	59.360	52.930	7.073	200.587	149.270	-29.657
1200	8.719	60.116	53.499	7.941	200.379	144.591	-26.333
1300	8.785	60.817	54.035	8.817	200.155	139.951	-23.528
1400	8.852	61.470	54.543	9.698	199.918	135.328	-21.125
1500	8.920	62.083	55.025	10.587	199.671	130.724	-19.046
1600	8.989	62.661	55.485	11.482	199.418	126.136	-17.229
1700	9.057	63.208	55.923	12.385	199.157	121.562	-15.628
1800	9.125	63.728	56.342	13.294	198.892	117.006	-14.206
1900	9.191	64.223	56.744	14.210	198.624	112.465	-12.936
2000	9.256	64.696	57.130	15.132	198.350	107.938	-11.795
2100	9.320	65.149	57.501	16.061	198.075	103.422	-10.763
2200	9.381	65.584	57.859	16.996	197.798	98.921	-9.827
2300	9.441	66.002	58.203	17.937	197.519	94.438	-8.974
2400	9.498	66.405	58.537	18.884	197.236	89.958	-8.192
2500	9.554	66.794	58.859	19.837	196.955	85.495	-7.474
2600	9.607	67.170	59.172	20.795	196.669	81.042	-6.812
2700	9.659	67.534	59.475	21.758	196.382	76.599	-6.200
2800	9.709	67.886	59.770	22.726	196.094	72.166	-5.633
2900	9.758	68.227	60.055	23.700	195.806	67.751	-5.106
3000	9.805	68.559	60.333	24.678	195.514	63.337	-4.614

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 7.622 + 0.786\times10^{-3}T + 2.183\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.622\times10^{-3}T + 0.393\times10^{-6}T^2 - 2.183\times10^{2}T^{-1} - 1.575$

2000-3000 K: $Cp^\circ = 8.627 + 0.428\times10^{-3}T - 9.124\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.627\times10^{-3}T + 0.214\times10^{-6}T^2 + 9.124\times10^{2}T^{-1} - 3.434$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 202.014 + 0.586\times10^{-3}T - 1.139\times10^{-6}T^2 - 562.900T^{-1}$

$\Delta Gf^\circ = 202.014 - 0.586\times10^{-3}T\ln T + 1.139\times10^{-6}T^2 - 281.450T^{-1} - 44.804\times10^{-3}T$

2000-3000 K: $\Delta Hf^\circ = 204.139 - 2.655\times10^{-3}T - 0.054\times10^{-6}T^2 - 527.600T^{-1}$

$\Delta Gf^\circ = 204.139 + 2.655\times10^{-3}T\ln T + 0.054\times10^{-6}T^2 - 263.800T^{-1} - 68.335\times10^{-3}T$

Source: Data from JANAF (51).

$C_3(g)$

Carbon (ideal triatomic gas)

[Formation: $3C(c) = C_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.020	56.677	56.677	0	196.000	180.329	-132.183
300	9.015	56.733	56.677	.017	196.005	180.232	-131.297
400	8.962	59.310	57.030	.912	196.168	174.944	-95.584
500	9.173	61.330	57.694	1.818	196.123	169.638	-74.148
600	9.490	63.029	58.446	2.750	195.924	164.360	-59.867
700	9.829	64.518	59.209	3.716	195.618	159.120	-49.679
800	10.153	65.852	59.957	4.716	195.241	153.933	-42.052
900	10.448	67.065	60.681	5.746	194.810	148.791	-36.131
1000	10.711	68.179	61.375	6.804	194.347	143.703	-31.406
1100	10.943	69.211	62.041	7.887	193.858	138.694	-27.556
1200	11.149	70.173	62.680	8.992	193.349	133.668	-24.344
1300	11.332	71.072	63.290	10.116	192.823	128.716	-21.639
1400	11.495	71.918	63.877	11.258	192.288	123.804	-19.326
1500	11.642	72.716	64.439	12.415	191.741	118.932	-17.328
1600	11.775	73.472	64.981	13.586	191.190	114.099	-15.585
1700	11.896	74.190	65.502	14.769	190.627	109.292	-14.050
1800	12.006	74.873	66.004	15.964	190.061	104.527	-12.691
1900	12.108	75.525	66.488	17.170	189.491	99.790	-11.478
2000	12.202	76.148	66.955	18.386	188.913	95.087	-10.390
2100	12.290	76.746	67.408	19.610	188.331	90.404	-9.408
2200	12.371	77.319	67.844	20.844	187.747	85.757	-8.519
2300	12.448	77.871	68.269	22.085	187.158	81.140	-7.710
2400	12.520	78.402	68.680	23.333	186.561	76.538	-6.970
2500	12.588	78.915	69.080	24.588	185.965	71.965	-6.291
2600	12.652	79.410	69.468	25.850	185.361	67.417	-5.667
2700	12.712	79.888	69.844	27.119	184.755	62.896	-5.091
2800	12.770	80.352	70.212	28.393	184.145	58.389	-4.557
2900	12.825	80.801	70.569	29.672	183.531	53.913	-4.063
3000	12.877	81.236	70.917	30.958	182.912	49.454	-3.603

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.030 + 2.378x10^{-3}T + 0.244x10^{5}T^{-2}$

$H°- H°_{298} = 8.030x10^{-3}T + 1.189x10^{-6}T^{2} - 0.244x10^{2}T^{-1} - 2.418$

2000-3000 K: $Cp° = 11.947 + 0.390x10^{-3}T - 211x10^{5}T^{-2}$

$H°- H°_{298} = 11.947x10^{-3}T + 0.195x10^{-6}T^{2} + 21.001x10^{2}T^{-1} - 7.338$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 198.667 - 2.524x10^{-3}T - 1.109x10^{-6}T^{2} - 541.300T^{-1}$

$\Delta Gf° = 198.667 + 2.524x10^{-3}T\ln T + 1.109x10^{-6}T^{2} - 270.650T^{-1} - 73.172x10^{-3}T$

2000-3000 K: $\Delta Hf° = 199.722 - 4.976x10^{-3}T - 0.207x10^{-6}T^{2} - 59.900T^{-1}$

$\Delta Gf° = 199.722 + 4.976x10^{-3}T\ln T + 0.207x10^{-6}T^{2} - 29.950T^{-1} - 90.593x10^{-3}T$

Source: Data from JANAF (51).

$C_4(g)$

Carbon (ideal tetratomic gas)

[Formation: $4C(c) = C_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	11.992	54.543	54.543	0	232.000	217.374	-159.338
300	12.031	54.618	54.545	.022	232.006	217.283	-158.288
400	13.780	58.333	55.038	1.318	232.326	212.326	-116.008
500	15.057	61.552	56.026	2.763	232.503	207.301	-90.610
600	16.045	64.388	57.188	4.320	232.552	202.257	-73.671
700	16.831	66.923	58.402	5.965	232.501	197.208	-61.570
800	17.463	69.213	59.612	7.681	232.381	192.175	-52.499
900	17.973	71.300	60.796	9.454	232.206	187.156	-45.447
1000	18.387	73.216	61.944	11.272	231.996	182.160	-39.811
1100	18.725	74.985	63.050	13.129	231.757	177.231	-35.212
1200	19.003	76.627	64.115	15.015	231.491	172.241	-31.369
1300	19.234	78.157	65.135	16.928	231.204	167.315	-28.128
1400	19.426	79.590	66.118	18.861	230.901	162.410	-25.353
1500	19.588	80.935	67.060	20.812	230.580	157.532	-22.952
1600	19.724	82.204	67.968	22.778	230.250	152.676	-20.854
1700	19.841	83.404	68.842	24.756	229.900	147.831	-19.005
1800	19.942	84.541	69.683	26.745	229.541	143.017	-17.364
1900	20.028	85.621	70.493	28.744	229.172	138.221	-15.899
2000	20.104	86.650	71.275	30.751	228.787	133.447	-14.582
2100	20.169	87.633	72.031	32.764	228.392	128.682	-13.392
2200	20.227	88.573	72.762	34.784	227.988	123.943	-12.312
2300	20.278	89.473	73.469	36.810	227.574	119.233	-11.330
2400	20.324	90.337	74.154	38.840	227.144	114.524	-10.429
2500	20.364	91.167	74.817	40.874	226.710	109.842	-9.602
2600	20.400	91.967	75.462	42.912	226.260	105.175	-8.841
2700	20.432	92.737	76.087	44.954	225.802	100.530	-8.137
2800	20.461	93.481	76.696	46.999	225.335	95.894	-7.485
2900	20.488	94.199	77.287	49.046	224.858	91.287	-6.879
3000	20.512	94.894	77.862	51.096	224.368	86.686	-6.315

*All data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 15.393 + 2.882\times10^{-3}T - 3.787\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.393\times10^{-3}T + 1.441\times10^{-6}T^2 + 3.787\times10^{2}T^{-1} - 5.988$

2000-3000 K: $Cp^\circ = 20.655 + 0.050\times10^{-3}T - 26.040\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 20.655\times10^{-3}T + 0.025\times10^{-6}T^2 + 26.040\times10^{2}T^{-1} - 11.961$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 232.792 + 1.321\times10^{-3}T - 1.623\times10^{-6}T^2 - 310.500T^{-1}$

$\Delta Gf^\circ = 232.792 - 1.321\times10^{-3}T\ln T + 1.623\times10^{-6}T^2 - 155.250T^{-1} - 42.922\times10^{-3}T$

2000-3000 K: $\Delta Hf^\circ = 234.787 - 1.909\times10^{-3}T - 0.511\times10^{-6}T^2 - 276.000T^{-1}$

$\Delta Gf^\circ = 234.787 + 1.909\times10^{-3}T\ln T + 0.511\times10^{-6}T^2 - 138.000T^{-1} - 66.250\times10^{-3}T$

Source: Data from JANAF (51) who estimated all except enthalpy of formation at 298 K.

$C_5(g)$

Carbon (ideal pentatomic gas)

[Formation: $5C(c) = C_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	14.611	57.806	57.806	0	234.000	218.810	-160.390
300	14.668	57.896	57.806	.027	234.007	218.716	-159.332
400	17.184	62.484	58.414	1.628	234.388	213.560	-116.682
500	18.964	66.520	59.640	3.440	234.615	208.323	-91.057
600	20.318	70.102	61.090	5.407	234.697	203.058	-73.963
700	21.385	73.317	62.611	7.494	234.664	197.783	-61.750
800	22.239	76.231	64.135	9.677	234.552	192.523	-52.594
900	22.927	78.891	65.629	11.936	234.376	187.274	-45.476
1000	23.484	81.337	67.079	14.258	234.163	182.051	-39.787
1100	23.940	83.597	68.479	16.630	233.915	176.905	-35.147
1200	24.314	85.697	69.828	19.043	233.638	171.680	-31.267
1300	24.624	87.656	71.125	21.490	233.335	166.527	-27.995
1400	24.883	89.490	72.371	23.966	233.016	161.399	-25.195
1500	25.101	91.215	73.571	26.466	232.676	156.296	-22.772
1600	25.286	92.841	74.725	28.985	232.325	151.219	-20.655
1700	25.444	94.378	75.836	31.522	231.952	146.156	-18.789
1800	25.579	95.837	76.908	34.073	231.568	141.123	-17.135
1900	25.696	97.223	77.940	36.637	231.172	136.109	-15.656
2000	25.798	98.543	78.937	39.212	230.757	131.121	-14.328
2100	25.886	99.804	79.901	41.796	230.331	126.142	-13.128
2200	25.965	101.010	80.833	44.389	229.894	121.192	-12.039
2300	26.033	102.166	81.736	46.989	229.444	116.270	-11.048
2400	26.095	103.275	82.610	49.595	228.975	111.351	-10.140
2500	26.149	104.342	83.459	52.207	228.502	106.459	-9.307
2600	26.198	105.368	84.281	54.825	228.010	101.590	-8.539
2700	26.241	106.358	85.081	57.447	227.507	96.738	-7.830
2800	26.281	107.313	85.858	60.073	226.993	91.899	-7.173
2900	26.316	108.236	86.614	62.703	226.468	87.091	-6.563
3000	26.349	109.129	87.350	65.336	225.926	82.289	-5.995

*All data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.564 + 3.816\times10^{-3}T - 5.416\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.564\times10^{-3}T + 1.908\times10^{-6}T^2 + 5.416\times10^{2}T^{-1} - 7.819$

2000-3000 K: $Cp^\circ = 26.531 + 0.070\times10^{-3}T - 34.919\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 26.531\times10^{-3}T + 0.035\times10^{-6}T^2 + 34.919\times10^{2}T^{-1} - 15.736$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 234.655 + 1.974\times10^{-3}T - 1.922\times10^{-6}T^2 - 319.900T^{-1}$

$\Delta Gf^\circ = 234.655 - 1.974\times10^{-3}T\ln T + 1.922\times10^{-6}T^2 - 159.950T^{-1} - 40.670\times10^{-3}T$

2000-3000 K: $\Delta Hf^\circ = 236.697 - 1.674\times10^{-3}T - 0.635\times10^{-6}T^2 - 108.100T^{-1}$

$\Delta Gf^\circ = 236.697 + 1.674\times10^{-3}T\ln T + 0.635\times10^{-6}T^2 - 54.050T^{-1} - 66.872\times10^{-3}T$

Source: Data from JANAF (51) who estimated all except enthalpy of formation at 298 K.

CO(g)

Carbon Monoxide (ideal gas)

[Formation: $C(c) + 0.5O_2(g) = CO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	6.965	47.217	47.217	0	-26.417	-32.780	24.028
300	6.965	47.260	47.217	.013	-26.414	-32.820	23.909
400	7.013	49.268	47.491	.711	-26.316	-34.972	19.107
500	7.121	50.844	48.010	1.417	-26.292	-37.140	16.234
600	7.276	52.155	48.593	2.137	-26.326	-39.306	14.317
700	7.450	53.290	49.186	2.873	-26.404	-41.465	12.946
800	7.624	54.296	49.762	3.627	-26.507	-43.609	11.913
900	7.786	55.203	50.317	4.397	-26.632	-45.741	11.107
1000	7.931	56.031	50.848	5.183	-26.766	-47.857	10.459
1100	8.057	56.793	51.354	5.983	-26.910	-49.948	9.924
1200	8.168	57.499	51.837	6.794	-27.060	-52.047	9.479
1300	8.263	58.157	52.299	7.616	-27.217	-54.123	9.099
1400	8.346	58.772	52.739	8.446	-27.378	-56.187	8.771
1500	8.417	59.351	53.161	9.285	-27.542	-58.240	8.485
1600	8.480	59.896	53.565	10.130	-27.709	-60.279	8.234
1700	8.535	60.412	53.953	10.980	-27.882	-62.312	8.011
1800	8.583	60.901	54.325	11.836	-28.057	-64.331	7.811
1900	8.626	61.366	54.683	12.697	-28.235	-66.340	7.631
2000	8.664	61.810	55.030	13.561	-28.419	-68.343	7.468
2100	8.698	62.233	55.362	14.430	-28.604	-70.333	7.320
2200	8.728	62.638	55.683	15.301	-28.794	-72.316	7.184
2300	8.756	63.027	55.994	16.175	-28.988	-74.289	7.059
2400	8.781	63.400	56.295	17.052	-29.187	-76.255	6.944
2500	8.804	63.759	56.587	17.931	-29.388	-78.212	6.837
2600	8.825	64.105	56.869	18.813	-29.593	-80.162	6.738
2700	8.844	64.438	57.143	19.696	-29.803	-82.102	6.646
2800	8.863	64.760	57.409	20.582	-30.015	-84.035	6.559
2900	8.879	65.072	57.669	21.469	-30.233	-85.960	6.478
3000	8.895	65.373	57.921	22.357	-30.455	-87.880	6.402

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.708 + 1.106\times10^{-3}T - 0.062\times10^{5}T^{-2}$

$H°- H°_{298} = 6.708\times10^{-3}T + 0.553\times10^{-6}T^{2} + 0.062\times10^{2}T^{-1} - 2.070$

2000-3000 K: $Cp° = 8.176 + 0.248\times10^{-3}T$

$H°- H°_{298} = 8.176\times10^{-3}T + 0.124\times10^{-6}T^{2} - 3.287$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -25.616 - 0.425\times10^{-3}T - 0.465\times10^{-6}T^{2} - 188.700T^{-1}$

$\Delta Gf° = -25.616 + 0.425\times10^{-3}T\ln T + 0.465\times10^{-6}T^{2} - 94.350T^{-1} - 25.527\times10^{-3}T$

2000-3000 K: $\Delta Hf° = -24.173 - 1.635\times10^{-3}T - 0.115\times10^{-6}T^{2} - 1035.000T^{-1}$

$\Delta Gf° = -24.173 + 1.635\times10^{-3}T\ln T + 0.115\times10^{-6}T^{2} - 517.500T^{-1} - 34.640\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (36). All other data from JANAF (51).

$CO_2(g)$

Carbon Dioxide (ideal gas)

[Formation: $C(c) + O_2(g) = CO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.874	51.070	51.070	0	-94.051	-94.258	69.092
300	8.896	51.125	51.072	.016	-94.052	-94.259	68.667
400	9.877	53.828	51.433	.958	-94.064	-94.326	51.537
500	10.666	56.120	52.146	1.987	-94.083	-94.389	41.257
600	11.310	58.124	52.979	3.087	-94.115	-94.447	34.402
700	11.846	59.908	53.844	4.245	-94.159	-94.499	29.504
800	12.293	61.520	54.704	5.453	-94.208	-94.545	25.828
900	12.667	62.990	55.543	6.702	-94.260	-94.584	22.968
1000	12.980	64.342	56.358	7.984	-94.312	-94.619	20.679
1100	13.243	65.592	57.141	9.296	-94.363	-94.636	18.802
1200	13.466	66.754	57.894	10.632	-94.413	-94.669	17.241
1300	13.656	67.839	58.617	11.988	-94.463	-94.688	15.918
1400	13.815	68.857	59.313	13.362	-94.512	-94.704	14.784
1500	13.953	69.815	59.982	14.750	-94.562	-94.717	13.800
1600	14.074	70.720	60.625	16.152	-94.611	-94.725	12.939
1700	14.177	71.576	61.244	17.565	-94.662	-94.730	12.178
1800	14.269	72.389	61.841	18.987	-94.715	-94.731	11.502
1900	14.352	73.163	62.417	20.418	-94.770	-94.732	10.897
2000	14.424	73.901	62.972	21.857	-94.828	-94.728	10.351
2100	14.489	74.606	63.509	23.303	-94.889	-94.721	9.858
2200	14.547	75.282	64.030	24.755	-94.953	-94.713	9.409
2300	14.600	75.929	64.532	26.212	-95.022	-94.698	8.998
2400	14.648	76.552	65.021	27.674	-95.096	-94.686	8.622
2500	14.692	77.151	65.495	29.141	-95.172	-94.667	8.276
2600	14.734	77.728	65.954	30.613	-95.253	-94.645	7.955
2700	14.771	78.284	66.400	32.088	-95.339	-94.618	7.659
2800	14.807	78.822	66.834	33.567	-95.429	-94.589	7.383
2900	14.841	79.342	67.256	35.049	-95.524	-94.555	7.126
3000	14.873	79.846	67.668	36.535	-95.624	-94.523	6.886

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.843 + 2.076\times10^{-3}T - 2.299\times10^{5}T^{-2}$

$H°- H°_{298} = 10.843\times10^{-3}T + 1.038\times10^{-6}T^{2} + 2.299\times10^{2}T^{-1} - 4.096$

2000-3000 K: $Cp° = 14.671 + 0.148\times10^{-3}T - 21.646\times10^{5}T^{-2}$

$H°- H°_{298} = 14.671\times10^{-3}T + 0.074\times10^{-6}T^{2} + 21.646\times10^{2}T^{-1} - 8.863$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -94.100 + 0.095\times10^{-3}T - 0.231\times10^{-6}T^{2} + 12.400T^{-1}$

$\Delta Gf° = -94.100 - 0.095\times10^{-3}T\ln T + 0.231\times10^{-6}T^{2} + 6.200T^{-1} - 0.125\times10^{-3}T$

2000-3000 K: $\Delta Hf° = -95.539 + 0.690\times10^{-3}T - 0.269\times10^{-6}T^{2} + 814.600T^{-1}$

$\Delta Gf° = -95.539 - 0.690\times10^{-3}T\ln T + 0.269\times10^{-6}T^{2} + 407.300T^{-1} + 4.941\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (36). All other data from JANAF (51).

Ca(c,1,g)

Calcium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.050	9.940	9.940	0
300	6.056	9.980	9.943	.011
400	6.275	11.750	10.182	.627
500	6.616	13.180	10.640	1.270
600	7.066	14.430	11.173	1.954
700	7.602	15.550	11.713	2.686
720	7.740	15.770	11.828	2.840
720	7.013	16.080	11.828	3.060
800	7.803	16.860	12.295	3.652
900	8.789	17.830	12.872	4.462
1000	9.776	18.810	13.400	5.410
1100	10.763	19.790	13.938	6.437
1112	10.880	19.900	13.995	6.567
1112	7.000	21.740	13.995	8.607
1200	7.000	22.270	14.584	9.223
1300	7.000	22.830	15.197	9.923
1400*	7.000	23.350	15.762	10.623
1500	7.000	23.830	16.281	11.323
1600	7.000	24.280	16.766	12.023
1700	7.000	24.710	17.226	12.723
1757	7.000	24.940	17.472	13.122
1757	4.979	45.786	17.472	49.748
1800	4.982	45.925	18.168	49.963
1900	4.992	46.195	19.636	50.462
2000	5.008	46.451	20.970	50.962

*Data extrapolated above 1300 K to 1757 K.

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-720 K: $Cp^\circ = 3.831 + 5.140\times10^{-3}T + 0.610\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 3.831\times10^{-3}T + 2.570\times10^{-6}T^2 - 0.610\times10^{2}T^{-1} - 1.166$

720-1112 K: $Cp^\circ = -0.107 + 9.884\times10^{-3}T$

$H^\circ - H^\circ_{298} = -0.107\times10^{-3}T + 4.942\times10^{-6}T^2 + 0.575$

1112-1757 K: $Cp^\circ = 7.000$

$H^\circ - H^\circ_{298} = 7.000\times10^{-3}T + 0.823$

1757-2000 K: $Cp^\circ = 4.970 + 0.014\times10^{-3}T$

$H^\circ - H^\circ_{298} = 4.970\times10^{-3}T + 0.007\times10^{-6}T^2 + 40.994$

Sources: Entropy for Ca(c) and enthalpy of formation of Ca(g) at 298 K from CODATA (36). Other data for Ca(c,1) from Hultgren (99), who extrapolated above 1300 K to boiling point by assuming constant heat capacity. Data for Ca(g) from JANAF (51).

Ca(g)

Calcium (ideal monatomic gas)

[Formation: Ca(c,l,g) = Ca(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	4.968	36.992	36.992	0	42.500	34.434	-25.241
300	4.968	37.023	36.993	.009	42.498	34.385	-25.049
400	4.968	38.452	37.187	.506	42.379	31.698	-17.319
500	4.968	39.560	37.554	1.003	42.233	29.043	-12.695
600	4.968	40.466	37.966	1.500	42.046	26.424	-9.625
700	4.968	41.232	38.381	1.996	41.810	23.833	-7.441
720	4.968	41.372	38.462	2.095	41.755	23.324	-7.080
720	4.968	41.372	38.462	2.095	41.535	23.324	-7.080
800	4.968	41.895	38.779	2.493	41.341	21.313	-5.822
900	4.968	42.480	39.158	2.990	41.028	18.843	-4.576
1000	4.968	43.004	39.517	3.487	40.577	16.383	-3.580
1100	4.968	43.477	39.855	3.984	40.047	13.991	-2.780
1112	4.968	43.531	39.895	4.044	39.977	13.702	-2.693
1112	4.968	43.531	39.895	4.044	37.937	13.702	-2.693
1200	4.968	43.910	40.177	4.480	37.757	11.789	-2.147
1300	4.968	44.307	40.479	4.977	37.554	9.634	-1.620
1400	4.969	44.675	40.765	5.474	37.351	7.496	-1.170
1500	4.970	45.018	41.037	5.971	37.148	5.366	-.782
1600	4.972	45.339	41.297	6.468	36.945	3.251	-.444
1700	4.976	45.641	41.544	6.965	36.742	1.159	-.149
1757	4.979	45.805	41.679	7.249	36.626	0	0
1757	4.979	45.805	41.679	7.249	0	0	0
1800	4.982	45.925	41.779	7.463	0	0	0
1900	4.992	46.195	42.004	7.962	0	0	0
2000	5.008	46.451	42.220	8.462	0	0	0

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 4.968$

$H^\circ - H^\circ_{298} = 4.968\times10^{-3}T - 1.481$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = 42.185 + 1.137\times10^{-3}T - 2.570\times10^{-6}T^2 + 61.000T^{-1}$

$\Delta Gf^\circ = 42.185 - 1.137\times10^{-3}T\ln T + 2.570\times10^{-6}T^2 + 30.500T^{-1} - 20.626\times10^{-3}T$

720-1112 K: $\Delta Hf^\circ = 40.444 + 5.075\times10^{-3}T - 4.942\times10^{-6}T^2$

$\Delta Gf^\circ = 40.444 - 5.075\times10^{-3}T\ln T + 4.942\times10^{-6}T^2 + 6.052\times10^{-3}T$

1112-1757 K: $\Delta Hf^\circ = 40.196 - 2.032\times10^{-3}T$

$\Delta Gf^\circ = 40.196 + 2.032\times10^{-3}T\ln T - 38.077\times10^{-3}T$

1757-2000 K: $\Delta Hf^\circ = 0$

$\Delta Gf^\circ = 0$

Sources: Enthalpy of formation at 298 K from CODATA (36). All other data from JANAF (51).

$Ca_2(g)$

Calcium (ideal diatomic gas)

[Formation: $2Ca(c,l,g) = Ca_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^{s}_{298})/T$	$H°-H^{s}_{298}$	ΔHf°	ΔGf°	
298.15	9.152	61.289	61.289	0	82.660	70.314	-51.541
300	9.145	61.345	61.289	.017	82.655	70.239	-51.169
400	8.699	63.918	61.643	.910	82.316	66.149	-36.142
500	8.270	65.811	62.295	1.758	81.878	62.153	-27.166
600	7.947	67.289	63.009	2.568	81.320	58.263	-21.222
700	7.716	68.495	63.709	3.350	80.638	54.461	-17.003
720	7.683	68.712	63.845	3.504	80.484	53.723	-16.307
720	7.683	68.712	63.845	3.504	80.044	53.723	-16.307
800	7.552	69.514	64.373	4.113	79.469	50.834	-13.887
900	7.433	70.397	64.995	4.862	78.598	47.335	-11.494
1000	7.344	71.175	65.574	5.601	77.441	43.886	-9.591
1100	7.278	71.872	66.116	6.332	76.118	40.597	-8.066
1112	7.272	71.951	66.178	6.419	75.945	40.200	-7.901
1112	7.272	71.951	66.178	6.419	71.865	40.200	-7.901
1200	7.226	72.503	66.622	7.057	71.271	37.715	-6.869
1300	7.186	73.079	67.097	7.777	70.591	34.946	-5.875
1400	7.154	73.611	67.544	8.494	69.908	32.233	-5.032
1500	7.128	74.103	67.964	9.208	69.222	29.558	-4.306
1600	7.107	74.563	68.363	9.920	68.534	26.929	-3.678
1700	7.089	74.993	68.740	10.630	67.844	24.370	-3.133
1757	7.081	75.227	68.947	11.034	67.450	22.916	-2.850
1757	7.081	75.227	68.947	11.034	-5.802	22.916	-2.850
1800	7.075	75.398	69.099	11.338	-5.928	23.686	-2.876
1900	7.062	75.780	69.441	12.045	-6.219	25.340	-2.915
2000	7.052	76.142	69.767	12.750	-6.514	27.006	-2.951

Phase changes: 720 K, α - β transition point of Ca; $\Delta H° = 0.220$ kcal/mol.
1112 K, melting point of Ca; $\Delta H° = 2.040$ kcal/mol.
1757 K, boiling point of Ca; $\Delta H° = 36.626$ kcal/mol of Ca.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.069 - 0.700\times10^{-3}T + 1.147\times10^{5}T^{-2}$

$H°-H^{s}_{298} = 8.069\times10^{-3}T - 0.350\times10^{-6}T^{2} - 1.147\times10^{2}T^{-1} - 1.990$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = 83.002 + 0.407\times10^{-3}T - 5.490\times10^{-6}T^{2} + 7.300T^{-1}$

$\Delta Gf° = 83.002 - 0.407\times10^{-3}T\ln T + 5.490\times10^{-6}T^{2} + 3.650T^{-1} - 41.916\times10^{-3}T$

720-1112 K: $\Delta Hf° = 79.520 + 8.283\times10^{-3}T - 10.234\times10^{-6}T^{2} - 114.700T^{-1}$

$\Delta Gf° = 79.520 - 8.283\times10^{-3}T\ln T + 10.234\times10^{-6}T^{2} - 57.350T^{-1} + 11.441\times10^{-3}T$

1112-1757 K: $\Delta Hf° = 79.024 - 5.931\times10^{-3}T - 0.350\times10^{-6}T^{2} - 114.700T^{-1}$

$\Delta Gf° = 79.024 + 5.931\times10^{-3}T\ln T + 0.350\times10^{-6}T^{2} - 57.350T^{-1} - 76.818\times10^{-3}T$

1757-2000 K: $\Delta Hf° = -1.318 - 1.871\times10^{-3}T - 0.364\times10^{-6}T^{2} - 114.700T^{-1}$

$\Delta Gf° = -1.318 + 1.871\times10^{-3}T\ln T + 0.364\times10^{-6}T^{2} - 57.350T^{-1} - 0.782\times10^{-3}T$

Source: Data from Chase (32).

CaO(c)

Calcium Oxide

[Formation: $Ca(c,l,g) + 0.5O_2(g) = CaO(c)$

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.050	9.100	9.100	0	-151.790	-144.234	105.725
300	10.081	9.162	9.100	.019	-151.788	-144.186	105.038
400	11.180	12.233	9.510	1.089	-151.689	-141.665	77.401
500	11.735	14.793	10.319	2.237	-151.550	-139.176	60.833
600	12.075	16.965	11.250	3.429	-151.419	-136.711	49.796
700	12.315	18.845	12.204	4.649	-151.320	-134.273	41.922
720	12.352	19.192	12.393	4.896	-151.307	-133.784	40.609
720	12.352	19.192	12.393	4.896	-151.527	-133.784	40.609
800	12.501	20.502	13.140	5.890	-151.444	-131.814	36.009
900	12.656	21.984	14.042	7.148	-151.404	-129.349	31.410
1000	12.793	23.325	14.904	8.421	-151.492	-126.912	27.736
1100	12.918	24.550	15.726	9.706	-151.654	-124.445	24.725
1112	12.932	24.690	15.822	9.861	-151.679	-124.153	24.400
1112	12.932	24.690	15.822	9.861	-153.719	-124.153	24.400
1200	13.035	25.679	16.509	11.004	-153.565	-121.819	22.186
1300	13.148	26.727	17.255	12.313	-153.384	-119.182	20.036
1400	13.256	27.705	17.967	13.633	-153.197	-116.556	18.195
1500	13.363	28.623	18.647	14.964	-153.000	-113.950	16.602
1600	13.468	29.489	19.298	16.306	-152.797	-111.356	15.210
1700	13.572	30.309	19.922	17.658	-152.586	-108.763	13.982
1757	13.631	30.757	20.266	18.433	-152.463	-107.296	13.346
1757	13.631	30.757	20.266	18.433	-189.089	-107.296	13.346
1800	13.676	31.087	20.520	19.020	-188.908	-105.264	12.781
1900	13.779	31.830	21.097	20.393	-188.481	-100.630	11.575
2000	13.882	32.539	21.651	21.776	-188.048	-96.018	10.492

Phase changes: 720 K, α - δ transition point of Ca; $\Delta H° = 0.220$ kcal/mol.
1112 K, melting point of Ca; $\Delta H° = 2.040$ kcal/mol.
1757 K, boiling point of Ca; $\Delta H° = 36.276$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.128 + 0.880\times10^{-3}T - 2.080\times10^{5}T^{-2}$

$H°- H°_{298} = 12.128\times10^{-3}T + 0.440\times10^{-6}T^2 + 2.080\times10^{2}T^{-1} - 4.353$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -153.801 + 4.682\times10^{-3}T - 2.382\times10^{-6}T^2 + 246.400T^{-1}$

$\Delta Gf° = -153.801 - 4.682\times10^{-3}T\ln T + 2.382\times10^{-6}T^2 + 123.200T^{-1} + 56.666\times10^{-3}T$

720-1112 K: $\Delta Hf° = -155.542 + 8.620\times10^{-3}T - 4.753\times10^{-6}T^2 + 185.400T^{-1}$

$\Delta Gf° = -155.542 - 8.620\times10^{-3}T\ln T + 4.753\times10^{-6}T^2 + 92.700T^{-1} + 83.345\times10^{-3}T$

1112-1757 K: $\Delta Hf° = -155.790 + 1.513\times10^{-3}T + 0.189\times10^{-6}T^2 + 185.400T^{-1}$

$\Delta Gf° = -155.790 - 1.513\times10^{-3}T\ln T - 0.189\times10^{-6}T^2 + 92.700T^{-1} + 39.215\times10^{-3}T$

1757-2000 K: $\Delta Hf° = -195.961 + 3.543\times10^{-3}T + 0.182\times10^{-6}T^2 + 185.400T^{-1}$

$\Delta Gf° = -195.961 - 3.543\times10^{-3}T\ln T - 0.182\times10^{-6}T^2 + 92.700T^{-1} + 77.233\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (36). Low-temperature heat capacities from Gmelin (78). High-temperature data based on Lander (141).

CaO(g)

Calcium Oxide (ideal gas)

[Formation: $Ca(c,l,g) + 0.5O_2(g) = CaO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.757	52.487	52.487	0	10.500	5.120	-3.753
300	7.765	52.535	52.488	.014	10.497	5.087	-3.706
400	8.147	54.824	52.797	.811	10.323	3.311	-1.809
500	8.398	56.671	53.393	1.639	10.142	1.577	-.689
600	8.564	58.218	54.071	2.488	9.929	-.114	.042
700	8.679	59.548	54.761	3.351	9.672	-1.773	.554
720	8.696	59.793	54.897	3.525	9.612	-2.095	.636
720	8.696	59.793	54.897	3.525	9.392	-2.095	.636
800	8.763	60.712	55.433	4.223	9.179	-3.359	.918
900	8.830	61.748	56.078	5.103	8.842	-4.891	1.188
1000	8.895	62.682	56.693	5.989	8.366	-6.411	1.401
1100	8.970	63.533	57.277	6.882	7.812	-7.860	1.562
1112	8.982	63.630	57.345	6.990	7.740	-8.036	1.579
1112	8.982	63.630	57.345	6.990	5.700	-8.036	1.579
1200	9.069	64.318	57.831	7.784	5.505	-9.116	1.660
1300	9.206	65.049	58.359	8.697	5.290	-10.327	1.736
1400	9.391	65.737	58.861	9.626	5.087	-11.518	1.798
1500	9.631	66.393	59.342	10.577	4.903	-12.702	1.851
1600	9.931	67.024	59.802	11.555	4.742	-13.873	1.895
1700	10.288	67.637	60.246	12.565	4.611	-15.024	1.931
1757	10.521	67.979	60.491	13.158	4.552	-15.682	1.951
1757	10.521	67.979	60.491	13.158	-32.074	-15.682	1.951
1800	10.697	68.236	60.673	13.614	-32.024	-15.248	1.851
1900	11.147	68.826	61.086	14.706	-31.878	-14.319	1.647
2000	11.626	69.410	61.488	15.844	-31.690	-13.402	1.464

Phase changes: 720 K, α - β transition point of Ca; $\Delta H° = 0.220$ kcal/mol.
1112 K, melting point of Ca; $\Delta H° = 2.040$ kcal/mol.
1757 K, boiling point of Ca; $\Delta H° = 36.626$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.025 + 1.084\times10^{-3}T - 0.526\times10^{5}T^{-2}$

$H°- H°_{298} = 8.025\times10^{-3}T + 0.542\times10^{-6}T^{2} + 0.526\times10^{2}T^{-1} - 2.617$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = 10.225 + 0.579\times10^{-3}T - 2.280\times10^{-6}T^{2} + 91.000T^{-1}$

$\Delta Gf° = 10.225 - 0.579\times10^{-3}T\ln T + 2.280\times10^{-6}T^{2} + 45.500T^{-1} - 15.014\times10^{-3}T$

720-1112 K: $\Delta Hf° = 8.484 + 4.517\times10^{-3}T - 4.651\times10^{-6}T^{2} + 30.000T^{-1}$

$\Delta Gf° = 8.484 - 4.517\times10^{-3}T\ln T + 4.651\times10^{-6}T^{2} + 15.000T^{-1} + 11.664\times10^{-3}T$

1112-1757 K: $\Delta Hf° = 8.236 - 2.590\times10^{-3}T + 0.291\times10^{-6}T^{2} + 30.000T^{-1}$

$\Delta Gf° = 8.236 + 2.590\times10^{-3}T\ln T - 0.291\times10^{-6}T^{2} + 15.000T^{-1} - 32.465\times10^{-3}T$

1757-2000 K: $\Delta Hf° = -31.935 - 0.560\times10^{-3}T + 0.284\times10^{-6}T^{2} + 30.000T^{-1}$

$\Delta Gf° = -31.935 + 0.560\times10^{-3}T\ln T - 0.284\times10^{-6}T^{2} + 15.000T^{-1} + 5.553\times10^{-3}T$

Source: Data from Chase (32).

Cd(c,l,g)

Cadmium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.200	12.380	12.380	0
300	6.210	12.420	12.383	.011
400	6.490	14.240	12.625	.646
500	6.780	15.720	13.100	1.310
594.26	7.060	16.910	13.611	1.960
594.26	7.100	19.400	13.611	3.440
600	7.100	19.480	13.675	3.483
700	7.100	20.570	14.580	4.193
800	7.100	21.520	15.391	4.903
900	7.100	22.360	16.123	5.613
1000	7.100	23.110	16.787	6.323
1040	7.100	23.380	17.027	6.607
1040	4.968	46.273	17.027	30.416
1100	4.968	46.551	18.630	30.713
1200	4.968	46.983	20.975	31.210
1300	4.968	47.381	22.991	31.707
1400	4.968	47.749	24.746	32.204
1500	4.968	48.092	26.291	32.701
1600	4.968	48.412	27.664	33.197
1700	4.968	48.714	28.894	33.694
1800	4.968	48.998	30.003	34.191
1900	4.968	49.266	31.009	34.688
2000	4.968	49.521	31.928	35.185

Phase changes: 594.26 K, melting point of Cd; ΔH° = 1.480 kcal/mol.
1040 K, boiling point of Cd; ΔH° = 23.809 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-594.26 K: $Cp^\circ = 5.319 + 2.892\times10^{-3}T + 0.016\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.319\times10^{-3}T + 1.446\times10^{-6}T^2 - 0.016\times10^{2}T^{-1} - 1.709$

594.26-1040 K: $Cp^\circ = 7.105$

$H^\circ - H^\circ_{298} = 7.105\times10^{-3}T - 0.782$

1040-2000 K: $Cp^\circ = 4.968$

$H^\circ - H^\circ_{298} = 4.968\times10^{-3}T + 25.249$

Sources: Data for Cd(c,l) from Hultgren (99). Enthalpy of formation at 298 K of Cd(g) from CODATA (37). Other data for Cd(g) from Hilsenrath (94).

Cd(g)

Cadmium (ideal monatomic gas)

[Formation: Cd(c,1,g) = Cd(g)]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^{\circ}_{298})/T$	$H°- H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	4.968	40.066	40.066	0	26.730	18.475	-13.543
300	4.968	40.097	40.067	.009	26.728	18.425	-13.422
400	4.968	41.526	40.261	.506	26.590	15.676	-8.565
500	4.968	42.634	40.628	1.003	26.423	12.966	-5.667
594.26	4.968	43.492	41.016	1.471	26.241	10.444	-3.841
594.26	4.968	43.492	41.016	1.471	24.761	10.444	-3.841
600	4.968	43.540	41.040	1.500	24.747	10.311	-3.756
700	4.968	44.306	41.455	1.996	24.533	7.918	-2.472
800	4.968	44.970	41.854	2.493	24.320	5.560	-1.519
900	4.968	45.555	42.233	2.990	24.107	3.232	-.785
1000	4.968	46.078	42.591	3.487	23.894	.926	-.202
1040	4.968	46.273	42.729	3.686	23.809	0	0
1040	4.968	46.273	42.729	3.686	0	0	0
1100	4.968	46.551	42.929	3.984	0	0	0
1200	4.968	46.983	43.250	4.480	0	0	0
1300	4.968	47.381	43.553	4.977	0	0	0
1400	4.968	47.749	43.839	5.474	0	0	0
1500	4.968	48.092	44.111	5.971	0	0	0
1600	4.968	48.412	44.369	6.468	0	0	0
1700	4.968	48.714	44.618	6.964	0	0	0
1800	4.968	48.998	44.853	7.461	0	0	0
1900	4.968	49.266	45.078	7.958	0	0	0
2000	4.968	49.521	45.293	8.455	0	0	0

Phase changes: 594.26 K, melting point of Cd; $\Delta H°$ = 1.480 kcal/mol.
1040 K, boiling point of Cd; $\Delta H°$ = 23.809 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.968$

$H°- H^{\circ}_{298} = 4.968\times10^{-3}T - 1.481$

Formation equations (kcal/mol):

298.15-594.26 K: $\Delta Hf° = 26.958 - 0.351\times10^{-3}T - 1.446\times10^{-6}T^2 + 1.600T^{-1}$

$\Delta Gf° = 26.958 + 0.351\times10^{-3}T\ln T + 1.446\times10^{-6}T^2 + 0.800T^{-1} - 30.890\times10^{-3}T$

594.26-1040 K: $\Delta Hf° = 26.031 - 2.137\times10^{-3}T$

$\Delta Gf° = 26.031 + 2.137\times10^{-3}T\ln T - 39.877\times10^{-3}T$

1040-2000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Sources: Enthalpy of formation at 298 K from CODATA (37). All other data from Hilsenrath (94).

CdO(c)

Cadmium Oxide

[Formation: $Cd(c,l,g) + 0.5O_2(g) = CdO(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.670	13.100	13.100	0	-61.700	-54.609	40.029
300	10.680	13.170	13.103	.020	-61.698	-54.565	39.750
400	11.410	16.350	13.528	1.129	-61.578	-52.204	28.523
500	11.830	18.950	14.366	2.292	-61.445	-49.880	21.802
594.26	12.103	21.014	15.258	3.420	-61.322	-47.709	17.546
594.26	12.103	21.014	15.258	3.420	-62.802	-47.709	17.546
600	12.120	21.130	15.313	3.490	-62.798	-47.558	17.323
700	12.360	23.040	16.304	4.715	-62.672	-45.047	14.064
800	12.570	24.680	17.229	5.961	-62.535	-42.519	11.615
900	12.760	26.170	18.139	7.228	-62.384	-40.020	9.718
1000	12.940	27.520	19.007	8.513	-62.223	-37.538	8.204
1040	13.008	28.029	19.344	9.032	-62.155	-36.561	7.683
1040	13.008	28.029	19.344	9.032	-85.964	-36.561	7.683
1100	13.110	28.770	19.847	9.815	-85.731	-33.727	6.701
1200	13.280	29.910	20.631	11.135	-85.332	-29.007	5.283
1300	13.440	30.980	21.386	12.472	-84.920	-24.330	4.090
1400	13.610	31.990	22.116	13.824	-84.496	-19.697	3.075
1500	13.770	32.930	22.801	15.193	-84.060	-15.077	2.197

Phase changes: 594.26 K, melting point of Cd; $\Delta H°$ = 1.480 kcal/mol.
1040 K, boiling point of Cd; $\Delta H°$ = 23.809 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 11.536 + 1.520\times10^{-3}T - 1.173\times10^{5}T^{-2}$

$H°- H°_{298} = 11.536\times10^{-3}T + 0.760\times10^{-6}T^{2} + 1.173\times10^{2}T^{-1} - 3.900$

Formation equations (kcal/mol):

298.15-594.26 K: $\Delta Hf° = -62.715 + 2.602\times10^{-3}T - 0.937\times10^{-6}T^{2} + 96.300T^{-1}$

$\Delta Gf° = -62.715 - 2.602\times10^{-3}T\ln T + 0.937\times10^{-6}T^{2} + 48.150T^{-1} + 41.192\times10^{-3}T$

594.26-1040 K: $\Delta Hf° = -63.642 + 0.816\times10^{-3}T + 0.509\times10^{-6}T^{2} + 94.700T^{-1}$

$\Delta Gf° = -63.642 - 0.816\times10^{-3}T\ln T - 0.509\times10^{-6}T^{2} + 47.350T^{-1} + 32.205\times10^{-3}T$

1040-1500 K: $\Delta Hf° = -89.674 + 2.953\times10^{-3}T + 0.509\times10^{-6}T^{2} + 94.700T^{-1}$

$\Delta Gf° = -89.674 - 2.953\times10^{-3}T\ln T - 0.509\times10^{-6}T^{2} + 47.350T^{-1} + 72.081\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (36). Other data from Mills (157).

Ce(c,1)

Cerium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.440	17.200	17.200	0
300	6.450	17.240	17.200	.012
400	6.760	19.140	17.460	.672
500	7.100	20.680	17.950	1.365
600	7.460	22.010	18.523	2.092
700	7.830	23.180	19.100	2.856
800	8.230	24.260	19.686	3.659
900	8.620	25.250	20.248	4.502
999	9.020	26.170	20.787	5.375
999	8.990	26.880	20.787	6.090
1000	8.990	26.890	20.791	6.099
1071	8.990	27.510	21.220	6.737
1071	9.010	28.730	21.220	8.042
1100	9.010	28.970	21.422	8.303
1200	9.010	29.750	22.080	9.204
1300	9.010	30.470	22.697	10.105
1400*	9.010	31.140	23.279	11.006
1500	9.010	31.760	23.822	11.907
1600	9.010	32.340	24.335	12.808
1700	9.010	32.890	24.826	13.709
1800	9.010	33.400	25.283	14.610
1900	9.010	33.890	25.726	15.511
2000	9.010	34.350	26.144	16.412

*Data above 1300 K extrapolated.

Phase changes: 999 K, γ - δ transition point of Ce; ΔH° = 0.715 kcal/mol.
1071 K, melting point of Ce; ΔH° = 1.305 kcal/mol.
3700 K, boiling point of Ce; ΔH° = 99.0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-999 K: $C_p^\circ = 5.085 + 3.894\times10^{-3}T + 0.172\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.085\times10^{-3}T + 1.947\times10^{-6}T^2 - 0.172\times10^{2}T^{-1} - 1.631$

999-1071 K: $C_p^\circ = 8.990$

$H^\circ - H^\circ_{298} = 8.990\times10^{-3}T - 2.891$

1071-2000 K: $C_p^\circ = 9.010$

$H^\circ - H^\circ_{298} = 9.010\times10^{-3}T - 1.608$

Sources: Entropy at 298 K from Parker (181). All other data from Hultgren (99) who extrapolated above 1300 K by assuming constant heat capacity.

Ce(g)

Cerium (ideal monatomic gas)

[Formation: Ce(c,l) = Ce(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.515	45.807	45.807	0	101.000	92.471	-67.782
300	5.519	45.841	45.808	.010	100.998	92.418	-67.325
400	5.876	47.472	46.027	.578	100.906	89.573	-48.940
500	6.401	48.838	46.456	1.191	100.826	86.747	-37.917
600	6.971	50.055	46.957	1.859	100.767	83.940	-30.575
700	7.517	51.171	47.480	2.584	100.728	81.134	-25.331
800	8.002	52.207	48.006	3.361	100.702	78.344	-21.402
900	8.408	53.174	48.527	4.182	100.680	75.548	-18.345
999	8.728	54.069	49.033	5.031	100.656	72.782	-15.922
999	8.728	54.069	49.033	5.031	99.941	72.782	-15.922
1000	8.731	54.078	49.038	5.040	99.941	72.753	-15.900
1071	8.904	54.683	49.392	5.667	99.930	70.828	-14.453
1071	8.904	54.683	49.392	5.667	98.625	70.828	-14.453
1100	8.974	54.922	49.535	5.926	98.623	70.076	-13.923
1200	9.146	55.710	50.017	6.832	98.628	67.476	-12.289
1300	9.257	56.447	50.483	7.753	98.648	64.878	-10.907
1400	9.322	57.136	50.935	8.682	98.676	62.282	-9.722
1500	9.350	57.780	51.369	9.616	98.709	59.679	-8.695
1600	9.354	58.384	51.790	10.551	98.743	57.073	-7.796
1700	9.339	58.950	52.194	11.486	98.777	54.475	-7.003
1800	9.315	59.484	52.585	12.419	98.809	51.858	-6.296
1900	9.285	59.987	52.961	13.349	98.838	49.254	-5.665
2000	9.253	60.462	53.324	14.276	98.864	46.640	-5.097

Phase changes: 999 K, γ - δ transition point of Ce; $\Delta H° = 0.715$ kcal/mol.
1071 K, melting point of Ce; $\Delta H° = 1.305$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.169 + 2.154\times10^{-3}T - 1.153\times10^{5}T^{-2}$

$H°- H°_{298} = 6.169\times10^{-3}T + 1.077\times10^{-6}T^{2} + 1.153\times10^{2}T^{-1} - 2.322$

Formation equations (kcal/mol):

298.15-999 K: $\Delta Hf° = 100.310 + 1.084\times10^{-3}T - 0.870\times10^{-6}T^{2} + 132.500T^{-1}$

$\Delta Gf° = 100.310 - 1.084\times10^{-3}T\ln T + 0.870\times10^{-6}T^{2} + 66.250T^{-1} - 21.120\times10^{-3}T$

999-1071 K: $\Delta Hf° = 101.570 - 2.821\times10^{-3}T + 1.077\times10^{-6}T^{2} + 115.300T^{-1}$

$\Delta Gf° = 101.570 + 2.821\times10^{-3}T\ln T - 1.077\times10^{-6}T^{2} + 57.650T^{-1} - 47.399\times10^{-3}T$

1071-2000 K: $\Delta Hf° = 100.286 - 2.841\times10^{-3}T + 1.077\times10^{-6}T^{2} + 115.300T^{-1}$

$\Delta Gf° = 100.286 + 2.841\times10^{-3}T\ln T - 1.077\times10^{-6}T^{2} + 57.650T^{-1} - 46.340\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). All other data from Hawkins (92).

$CeO_2(c)$

Cerium Dioxide

[Formation: $Ce(c,l) + O_2(g) = CeO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	14.730	14.890	14.890	0	-260.200	-244.900	179.515
300	14.762	14.981	14.891	.027	-260.198	-244.806	178.338
400	16.035	19.409	15.487	1.569	-260.026	-239.698	130.963
500	16.908	23.086	16.648	3.219	-259.800	-234.643	102.561
600	17.528	26.227	17.989	4.943	-259.558	-229.630	83.642
700	17.983	28.965	19.366	6.719	-259.324	-224.666	70.143
800	18.326	31.389	20.719	8.536	-259.108	-219.723	60.025
900	18.593	33.564	22.028	10.382	-258.919	-214.815	52.163
999	18.808	35.515	23.270	12.233	-258.759	-209.975	45.935
999	18.808	35.515	23.270	12.233	-259.474	-209.975	45.935
1000	18.810	35.534	23.282	12.252	-259.473	-209.927	45.879
1071	18.946	36.829	24.137	13.593	-259.365	-206.407	42.119
1071	18.946	36.829	24.137	13.593	-260.670	-206.407	42.119
1100	19.001	37.336	24.479	14.143	-260.625	-204.939	40.717
1200	19.183	38.997	25.620	16.052	-260.465	-199.888	36.404
1300	19.370	40.540	26.709	17.980	-260.294	-194.848	32.757
1400	19.574	41.983	27.749	19.927	-260.112	-189.818	29.632
1500	19.802	43.341	28.744	21.895	-259.915	-184.807	26.926
1600	20.059	44.627	29.697	23.888	-259.700	-179.809	24.560
1700	20.348	45.852	30.612	25.908	-259.463	-174.817	22.474
1800	20.667	47.024	31.491	27.959	-259.201	-169.853	20.623
1900	21.012	48.150	32.338	30.043	-258.912	-164.891	18.966
2000	21.378	49.237	33.156	32.162	-258.593	-159.955	17.479

Phase changes: 999 K, γ - δ transition point of Ce; $\Delta H° = 0.715$ kcal/mol.
1071 K, melting point of Ce: $\Delta H° = 1.305$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 16.761 + 2.216\times10^{-3}T - 2.392\times10^{5}T^{-2}$

$H°-H°_{298} = 16.761\times10^{-3}T + 1.108\times10^{-6}T^{2} + 2.392\times10^{2}T^{-1} - 5.898$

Formation equations (kcal/mol):

298.15-999 K: $\Delta Hf° = -262.115 + 4.446\times10^{-3}T - 1.342\times10^{-6}T^{2} + 211.200T^{-1}$

$\Delta Gf° = -262.115 - 4.446\times10^{-3}T\ln T + 1.342\times10^{-6}T^{2} + 105.600T^{-1} + 81.480\times10^{-3}T$

999-1071 K: $\Delta Hf° = -260.854 + 0.541\times10^{-3}T + 0.605\times10^{-6}T^{2} + 194.000T^{-1}$

$\Delta Gf° = -260.854 - 0.541\times10^{-3}T\ln T - 0.605\times10^{-6}T^{2} + 97.000T^{-1} + 55.201\times10^{-3}T$

1071-2000 K: $\Delta Hf° = -262.138 + 0.521\times10^{-3}T + 0.605\times10^{-6}T^{2} + 194.000T^{-1}$

$\Delta Gf° = -262.138 - 0.521\times10^{-3}T\ln T - 0.605\times10^{-6}T^{2} + 97.000T^{-1} + 56.260\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). Low-temperature heat capacities and entropy at 298 K from Westrum (245). High-temperature data based on King (130).

$Ce_2O_3(c)$

Dicerium Trioxide, Cerium Sesquioxide

[Formation: $2Ce(c) + 1.5O_2(g) = Ce_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	28.090	35.400	35.400	0	-429.300	-407.682	298.835
300	28.157	35.574	35.401	.052	-429.291	-407.548	296.894
400	30.661	44.063	36.541	3.009	-428.719	-400.379	218.754
500	32.020	51.063	38.767	6.148	-428.063	-393.374	171.941
600	32.964	56.988	41.323	9.399	-427.398	-386.492	140.778
700	33.741	62.129	43.935	12.736	-426.757	-379.734	118.557
800	34.453	66.681	46.500	16.145	-426.151	-373.047	101.910
900	35.152	70.780	48.973	19.626	-425.576	-366.448	88.985
999	35.854	74.484	51.321	23.140	-425.036	-359.979	78.751
999	35.854	74.484	51.321	23.140	-426.466	-359.979	78.751
1000	35.861	74.520	51.344	23.176	-426.461	-359.916	78.659

Phase change: 999 K, γ - δ transition point of Ce; $\Delta H° = 0.715$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 31.358 + 4.664\times10^{-3}T - 4.142\times10^{5}T^{-2}$

$H°- H°_{298} = 31.358\times10^{-3}T + 2.332\times10^{-6}T^2 + 4.142\times10^{2}T^{-1} - 10.946$

Formation equations (kcal/mol):

298.15-999 K: $\Delta Hf° = -433.455 + 10.343\times10^{-3}T - 2.316\times10^{-6}T^2 + 380.800T^{-1}$

$\Delta Gf° = -433.455 - 10.343\times10^{-3}T\ln T + 2.316\times10^{-6}T^2 + 190.400T^{-1} + 142.541\times10^{-3}T$

999-1000 K: $\Delta Hf° = -430.935 + 2.533\times10^{-3}T + 1.578\times10^{-6}T^2 + 346.400T^{-1}$

$\Delta Gf° = -430.935 - 2.533\times10^{-3}T\ln T - 1.578\times10^{-6}T^2 + 173.200T^{-1} + 89.984\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). Low-temperature heat capacities and entropy at 298 K from Justice (111). High-temperature data based on Pankratz (176).

$Cl_2(g)$

Chlorine

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	8.111	53.290	53.290	0
300	8.119	53.340	53.290	.015
400	8.437	55.725	53.612	.845
500	8.624	57.629	54.233	1.698
600	8.741	59.213	54.935	2.567
700	8.821	60.566	55.645	3.445
800	8.878	61.748	56.334	4.331
900	8.922	62.797	56.996	5.221
1000	8.956	63.738	57.623	6.115
1100	8.985	64.593	58.218	7.012
1200	9.010	65.376	58.783	7.912
1300	9.032	66.098	59.318	8.814
1400	9.051	66.768	59.827	9.718
1500	9.069	67.393	60.310	10.624
1600	9.086	67.979	60.771	11.532
1700	9.102	68.531	61.213	12.441
1800	9.117	69.051	61.633	13.352
1900	9.133	69.545	62.038	14.264
2000	9.149	70.014	62.424	15.179
2100	9.166	70.460	62.796	16.094
2200	9.184	70.887	63.154	17.012
2300	9.203	71.296	63.500	17.931
2400	9.223	71.688	63.833	18.852
2500	9.245	72.065	64.155	19.776
2600	9.268	72.428	64.466	20.701
2700	9.293	72.778	64.767	21.629
2800	9.319	73.117	65.060	22.560
2900	9.346	73.444	65.343	23.493
3000	9.374	73.761	65.618	24.429

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 8.827 + 0.176\times10^{-3}T - 0.683\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.827\times10^{-3}T + 0.088\times10^{-6}T^2 + 0.683\times10^{2}T^{-1} - 2.869$

Sources: Entropy at 298 K from CODATA (36). All other data from JANAF (51).

Cl(g)

Chlorine (ideal monatomic gas)

[Formation: $0.5Cl_2(g) = Cl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.219	39.454	39.454	0	28.992	25.173	-18.452
300	5.223	39.487	39.454	.010	28.995	25.149	-18.321
400	5.370	41.011	39.661	.540	29.110	23.850	-13.031
500	5.436	42.218	40.056	1.081	29.224	22.522	-9.844
600	5.445	43.210	40.502	1.625	29.333	21.171	-7.712
700	5.424	44.048	40.949	2.169	29.439	19.803	-6.183
800	5.389	44.771	41.383	2.710	29.537	18.419	-5.032
900	5.351	45.403	41.795	3.247	29.629	17.024	-4.134
1000	5.314	45.965	42.185	3.780	29.715	15.618	-3.413
1100	5.279	46.470	42.553	4.309	29.795	14.204	-2.822
1200	5.248	46.928	42.898	4.836	29.872	12.784	-2.328
1300	5.221	47.347	43.225	5.359	29.944	11.357	-1.909
1400	5.196	47.733	43.533	5.880	30.013	9.924	-1.549
1500	5.175	48.090	43.824	6.399	30.079	8.489	-1.237
1600	5.156	48.424	44.102	6.915	30.141	7.046	-.962
1700	5.140	48.736	44.365	7.430	30.202	5.602	-.720
1800	5.125	49.029	44.616	7.943	30.259	4.153	-.504
1900	5.112	49.306	44.856	8.455	30.315	2.701	-.311
2000	5.101	49.568	45.086	8.965	30.368	1.245	-.136
2100	5.090	49.816	45.304	9.475	30.420	-0.211	.022
2200	5.081	50.053	45.515	9.984	30.470	-1.671	.166
2300	5.073	50.279	45.718	10.491	30.518	-3.134	.298
2400	5.066	50.495	45.912	10.998	30.564	-4.598	.419
2500	5.059	50.701	46.099	11.504	30.608	-6.063	.530
2600	5.053	50.899	46.280	12.010	30.652	-7.529	.633
2700	5.048	51.090	46.455	12.515	30.693	-9.000	.729
2800	5.043	51.274	46.624	13.020	30.732	-10.471	.817
2900	5.038	51.450	46.787	13.524	30.770	-11.942	.900
3000	5.034	51.621	46.945	14.027	30.805	-13.417	.977

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 5.723 - 0.344x10^{-3}T - 0.357x10^{5}T^{-2}$

$H°- H°_{298} = 5.723x10^{-3}T - 0.172x10^{-6}T^{2} + 0.357x10^{2}T^{-1} - 1.811$

2000-3000 K: $Cp° = 5.519 - 0.156x10^{-3}T - 4.235x10^{5}T^{-2}$

$H°- H°_{298} = 5.519x10^{-3}T - 0.078x10^{-6}T^{2} + 4.235x10^{2}T^{-1} - 1.973$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 28.616 + 1.310x10^{-3}T - 0.216x10^{-6}T^{2} + 1.550T^{-1}$

$\Delta Gf° = 28.616 - 1.310x10^{-3}T\ln T + 0.216x10^{-6}T^{2} + 0.775T^{-1} - 4.159x10^{-3}T$

2000-3000 K: $\Delta Hf° = 28.454 + 1.105x10^{-3}T - 0.122x10^{-6}T^{2} + 389.350T^{-1}$

$\Delta Gf° = 28.454 - 1.105x10^{-3}T\ln T + 0.122x10^{-6}T^{2} + 194.675T^{-1} - 5.489x10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (36). All other data from Chase (31).

ClO(g)

Chlorine Oxide (ideal gas)

[Formation: $0.5Cl_2(g) + 0.5O_2(g) = ClO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.540	54.145	54.145	0	24.340	23.446	-17.186
300	7.548	54.191	54.145	.014	24.340	23.441	-17.077
400	7.942	56.419	54.446	.789	24.345	23.140	-12.643
500	8.229	58.224	55.026	1.599	24.363	22.839	-9.983
600	8.429	59.743	55.690	2.432	24.384	22.531	-8.207
700	8.571	61.054	56.364	3.283	24.407	22.221	-6.938
800	8.676	62.205	57.024	4.145	24.427	21.906	-5.984
900	8.754	63.232	57.658	5.017	24.447	21.590	-5.243
1000	8.816	64.158	58.263	5.895	24.465	21.271	-4.649
1100	8.865	65.000	58.836	6.780	24.482	20.952	-4.163
1200	8.906	65.773	59.383	7.668	24.495	20.630	-3.757
1300	8.941	66.488	59.903	8.561	24.510	20.307	-3.414
1400	8.971	67.151	60.397	9.456	24.521	19.984	-3.120
1500	8.998	67.771	60.868	10.355	24.531	19.659	-2.864
1600	9.022	68.353	61.318	11.256	24.540	19.334	-2.641
1700	9.044	68.900	61.748	12.159	24.548	19.010	-2.444
1800	9.064	69.418	62.160	13.065	24.554	18.683	-2.268
1900	9.083	69.909	62.555	13.972	24.558	18.356	-2.111
2000	9.100	70.375	62.935	14.881	24.560	18.030	-1.970

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.333 + 0.506x10^{-3}T - 0.840x10^{5}T^{-2}$

$H°- H°_{298} = 8.333x10^{-3}T + 0.253x10^{-6}T^{2} + 0.840x10^{2}T^{-1} - 2.789$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 24.162 + 0.305x10^{-3}T - 0.042x10^{-6}T^{2} + 27.250T^{-1}$

$\Delta Gf° = 24.162 - 0.305x10^{-3}T\ln T + 0.042x10^{-6}T^{2} + 13.625T^{-1} - 0.830x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from JANAF (51).

$Cl_2O(g)$

Dichlorine Oxide (ideal gas)

[Formation: $Cl_2(g) + 0.5O_2(g) = Cl_2O(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.427	64.019	64.019	0	19.200	23.307	-17.084
300	11.447	64.090	64.020	.021	19.200	23.332	-16.997
400	12.280	67.508	64.481	1.211	19.205	24.709	-13.500
500	12.777	70.306	65.374	2.466	19.241	26.083	-11.401
600	13.086	72.665	66.398	3.760	19.289	27.446	-9.997
700	13.287	74.698	67.441	5.080	19.342	28.803	-8.992
800	13.424	76.482	68.462	6.416	19.393	30.149	-8.236
900	13.521	78.069	69.443	7.763	19.443	31.491	-7.647
1000	13.592	79.497	70.378	9.119	19.491	32.827	-7.174
1100	13.645	80.795	71.267	10.481	19.537	34.159	-6.787
1200	13.686	81.984	72.111	11.848	19.580	35.487	-6.463
1300	13.719	83.081	72.913	13.218	19.620	36.810	-6.188
1400	13.745	84.099	73.677	14.591	19.656	38.130	-5.952
1500	13.766	85.048	74.403	15.967	19.691	39.449	-5.748
1600	13.783	85.937	75.097	17.344	19.722	40.764	-5.568
1700	13.797	86.773	75.759	18.723	19.751	42.080	-5.410
1800	13.809	87.562	76.394	20.103	19.776	43.392	-5.268
1900	13.820	88.309	77.001	21.485	19.799	44.705	-5.142
2000	13.829	89.018	77.584	22.867	19.817	46.015	-5.028

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.320 + 0.388\times10^{-3}T - 1.786\times10^{5}T^{-2}$

$H°- H°_{298} = 13.320\times10^{-3}T + 0.194\times10^{-6}T^{2} + 1.786\times10^{2}T^{-1} - 4.588$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 18.657 + 0.878\times10^{-3}T - 0.145\times10^{-6}T^{2} + 87.700T^{-1}$

$\Delta Gf° = 18.657 - 0.878\times10^{-3}T\ln T + 0.145\times10^{-6}T^{2} + 43.850T^{-1} + 20.061\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from JANAF (51).

Cm(c,1)

Curium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15*	6.617	17.200	17.200	0
300	6.621	17.241	17.201	.012
400	6.828	19.174	17.462	.685
500	7.035	20.720	17.964	1.378
600	7.242	22.021	18.534	2.092
700	7.449	23.153	19.116	2.826
800	7.656	24.161	19.685	3.581
900	7.863	25.075	20.234	4.357
1000	8.070	25.914	20.760	5.154
1100	8.277	26.693	21.265	5.971
1200	8.484	27.422	21.748	6.809
1300	8.691	28.109	22.211	7.668
1400	8.898	28.761	22.655	8.548
1500	9.105	29.382	23.083	9.448
1550	9.208	29.682	23.291	9.906
1550	8.000	30.182	23.291	10.681
1600	8.000	30.436	23.510	11.081
1618	8.000	30.525	23.587	11.225
1618	9.600	32.688	23.587	14.725
1700	9.600	33.163	24.038	15.512
1800	9.600	33.712	24.561	16.472
1900	9.600	34.231	25.056	17.432
2000	9.600	34.723	25.527	18.392

*All data except temperature of fusion estimated.

Phase changes: 1550 K, α - β transition point of Cm; ΔH° = 0.775 kcal/mol.
1618 K, melting point of Cm; ΔH° = 3.500 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1550 K: $C_p^\circ = 5.998 + 2.072\times10^{-3}T + 0.001\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.998\times10^{-3}T + 1.036\times10^{-6}T^{2} - 0.001\times10^{2}T^{-1} - 1.880$

1550-1618 K: $C_p^\circ = 8.000$

$H^\circ - H^\circ_{298} = 8.000\times10^{-3}T - 1.719$

1618-2000 K: $C_p^\circ = 9.600$

$H^\circ - H^\circ_{298} = 9.600\times10^{-3}T - 0.808$

Source: Data from Oetting (167) who estimated all except temperature of fusion.

Cm(g)

Curium (ideal monatomic gas)

[Formation: Cm(c,l) = Cm(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH_f°	ΔG_f°	
298.15	6.717	47.158	47.158	0	92.600	83.668	-61.330
300	6.723	47.200	47.160	.012	92.600	83.612	-60.911
400	6.936	49.168	47.425	.697	92.612	80.614	-44.045
500	6.962	50.721	47.935	1.393	92.615	77.614	-33.925
600	6.858	51.983	48.508	2.085	92.593	74.616	-27.178
700	6.705	53.029	49.082	2.763	92.537	71.624	-22.362
800	6.555	53.914	49.632	3.426	92.445	68.643	-18.752
900	6.429	54.678	50.150	4.075	92.318	65.675	-15.948
1000	6.334	55.351	50.638	4.713	92.159	62.722	-13.708
1100	6.266	55.951	51.094	5.343	91.972	59.788	-11.879
1200	6.223	56.494	51.521	5.967	91.758	56.872	-10.358
1300	6.199	56.991	51.923	6.588	91.520	53.973	-9.074
1400	6.191	57.450	52.302	7.207	91.259	51.094	-7.976
1500	6.196	57.878	52.660	7.827	90.979	48.235	-7.028
1550	6.204	58.081	52.831	8.137	90.831	46.812	-6.600
1550	6.204	58.081	52.831	8.137	90.056	46.812	-6.600
1600	6.212	58.278	52.999	8.447	89.966	45.419	-6.204
1618	6.216	58.348	53.058	8.559	89.934	44.917	-6.067
1618	6.216	58.348	53.058	8.559	86.434	44.917	-6.067
1700	6.236	58.655	53.320	9.069	86.157	42.821	-5.505
1800	6.269	59.012	53.626	9.694	85.822	40.282	-4.891
1900	6.308	59.352	53.919	10.323	85.491	37.761	-4.343
2000	6.354	59.677	54.199	10.956	85.164	35.256	-3.853

Phase changes: 1550 K, α - β transition point of Cm; ΔH° = 0.775 kcal/mol.
1618 K, melting point of Cm; ΔH° = 3.500 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 7.283 - 0.712\times10^{-3}T - 0.314\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.283\times10^{-3}T - 0.356\times10^{-6}T^2 + 0.314\times10^{2}T^{-1} - 2.245$

Formation equations (kcal/mol):

298.15-1550 K: $\Delta H_f^\circ = 92.235 + 1.285\times10^{-3}T - 1.392\times10^{-6}T^2 + 31.500T^{-1}$

$\Delta G_f^\circ = 92.235 - 1.285\times10^{-3}T\ln T + 1.392\times10^{-6}T^2 + 15.750T^{-1} - 22.004\times10^{-3}T$

1550-1618 K: $\Delta H_f^\circ = 92.074 - 0.717\times10^{-3}T - 0.356\times10^{-6}T^2 + 31.400T^{-1}$

$\Delta G_f^\circ = 92.074 + 0.717\times10^{-3}T\ln T + 0.356\times10^{-6}T^2 + 15.700T^{-1} - 35.002\times10^{-3}T$

1618-2000 K: $\Delta H_f^\circ = 91.163 - 2.317\times10^{-3}T - 0.356\times10^{-6}T^2 + 31.400T^{-1}$

$\Delta G_f^\circ = 91.163 + 2.317\times10^{-3}T\ln T + 0.356\times10^{-6}T^2 + 15.700T^{-1} - 46.261\times10^{-3}T$

Source: Data from Oetting (167).

Co(c,l)

Cobalt

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.930	7.180	7.180	0
300	5.940	7.220	7.183	.011
400	6.340	8.970	7.408	.625
500	6.740	10.440	7.880	1.280
600	7.090	11.700	8.413	1.972
700	7.420	12.820	8.961	2.700
700	7.310	12.970	8.961	2.808
800	7.750	13.980	9.530	3.560
900	8.250	14.920	10.076	4.360
1000	8.840	15.810	10.596	5.214
1100	9.520	16.690	11.116	6.131
1200	10.330	17.550	11.615	7.122
1300	11.630	18.420	12.102	8.213
1394	13.140	19.280	12.552	9.379
1400	10.570	19.330	12.581	9.448
1500	9.500	20.010	13.051	10.438
1600	9.150	20.610	13.505	11.368
1700	9.030	21.160	13.939	12.276
1768	9.020	21.510	14.221	12.890
1768	11.516	23.604	14.221	16.590
1800	11.516	23.811	14.389	16.959
1900	11.516	24.433	14.901	18.110
2000	11.516	25.024	15.393	19.262
2100	11.516	25.586	15.865	20.414
2200	11.516	26.122	16.320	21.565
2300	11.516	26.633	16.756	22.717
2400	11.516	27.124	17.179	23.869
2500	11.516	27.594	17.586	25.020

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
1394 K, Curie temperature of Co; ΔH° = 0 kcal/mol.
1768 K, melting point of Co; ΔH° = 3.700 kcal/mol.
3200 K, boiling point of Co; ΔH° = 90.0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp^\circ = 5.001 + 3.554\times10^{-3}T - 0.116\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.001\times10^{-3}T + 1.777\times10^{-6}T^2 + 0.116\times10^{2}T^{-1} - 1.688$

700-1394 K: $Cp^\circ = -3.485 + 10.830\times10^{-3}T + 15.748\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = -3.485\times10^{-3}T + 5.415\times10^{-6}T^2 - 15.748\times10^{2}T^{-1} + 4.844$

1394-1768 K: $Cp^\circ = 14.425 - 3.186\times10^{-3}T$

$H^\circ - H^\circ_{298} = 14.425\times10^{-3}T - 1.593\times10^{-6}T^2 - 7.634$

1768-2500 K: $Cp^\circ = 11.516$

$H^\circ - H^\circ_{298} = 11.516\times10^{-3}T - 3.770$

Sources: Data for Co(c) from Hultgren (99). Data for Co(l) based on Treverton (225).

Co(g)

Cobalt (ideal monatomic gas)

[Formation: Co(c,l) = Co(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	$C_p°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta H_f°$	$\Delta G_f°$	
298.15	5.503	42.879	42.879	0	101.500	90.856	-66.599
300	5.510	42.913	42.880	.010	101.499	90.791	-66.140
400	5.857	44.548	43.101	.579	101.454	87.223	-47.656
500	6.077	45.881	43.527	1.177	101.397	83.677	-36.575
600	6.188	47.000	44.015	1.791	101.319	80.139	-29.190
700	6.236	47.958	44.511	2.413	101.213	76.616	-23.920
700	6.236	47.958	44.511	2.413	101.105	76.616	-23.920
800	6.259	48.793	44.995	3.038	100.978	73.128	-19.977
900	6.274	49.531	45.460	3.664	100.804	69.654	-16.914
1000	6.291	50.193	45.901	4.292	100.578	66.195	-14.467
1100	6.309	50.793	46.318	4.922	100.291	62.778	-12.473
1200	6.329	51.343	46.715	5.554	99.932	59.380	-10.815
1300	6.347	51.850	47.090	6.188	99.475	56.016	-9.417
1394	6.362	52.294	47.426	6.786	98.907	52.886	-8.291
1400	6.363	52.321	47.447	6.824	98.876	52.689	-8.225
1500	6.375	52.761	47.787	7.461	98.523	49.396	-7.197
1600	6.383	53.172	48.110	8.099	98.231	46.132	-6.301
1700	6.386	53.559	48.420	8.737	97.961	42.883	-5.513
1768	6.385	53.809	48.622	9.172	97.782	40.677	-5.028
1768	6.385	53.809	48.622	9.172	94.082	40.677	-5.028
1800	6.385	53.924	48.715	9.376	93.917	39.714	-4.822
1900	6.381	54.270	48.999	10.014	93.404	36.714	-4.223
2000	6.374	54.597	49.271	10.652	92.890	33.744	-3.687

Phase changes: 700 K, α - β transition point of Co; $\Delta H°$ = 0.108 kcal/mol.
1394 K, Curie temperature of Co; $\Delta H°$ = 0 kcal/mol.
1768 K, melting point of Co; $\Delta H°$ = 3.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p° = 6.357 + 0.028\times10^{-3}T - 0.767\times10^{5}T^{-2}$

$H°- H°_{298} = 6.357\times10^{-3}T + 0.014\times10^{-6}T^2 + 0.767\times10^{2}T^{-1} - 2.154$

Formation equations (kcal/mol):

298.15-700 K: $\Delta H_f° = 101.034 + 1.356\times10^{-3}T - 1.763\times10^{-6}T^2 + 65.100T^{-1}$

$\Delta G_f° = 101.034 - 1.356\times10^{-3}T\ln T + 1.763\times10^{-6}T^2 + 32.550T^{-1} - 27.302\times10^{-3}T$

700-1394 K: $\Delta H_f° = 94.502 + 9.842\times10^{-3}T - 5.401\times10^{-6}T^2 + 1651.500T^{-1}$

$\Delta G_f° = 94.502 - 9.842\times10^{-3}T\ln T + 5.401\times10^{-6}T^2 + 825.750T^{-1} + 33.456\times10^{-3}T$

1394-1768 K: $\Delta H_f° = 106.980 - 8.068\times10^{-3}T + 1.607\times10^{-6}T^2 + 76.700T^{-1}$

$\Delta G_f° = 106.980 + 8.068\times10^{-3}T\ln T - 1.607\times10^{-6}T^2 + 38.350T^{-1} - 94.988\times10^{-3}T$

1768-2000 K: $\Delta H_f° = 103.117 - 5.159\times10^{-3}T + 0.014\times10^{-6}T^2 + 76.700T^{-1}$

$\Delta G_f° = 103.117 + 5.159\times10^{-3}T\ln T - 0.014\times10^{-6}T^2 + 38.350T^{-1} - 73.867\times10^{-3}T$

Source: Data from JANAF (51).

CoO(c)

Cobalt Oxide

[Formation: $Co(c,l) + 0.5O_2(g) = CoO(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.200	12.660	12.660	0	-56.870	-51.198	37.529
300	13.161	12.742	12.662	.024	-56.864	-51.163	37.272
400	12.602	16.397	13.162	1.294	-56.563	-49.315	26.944
500	12.833	19.233	14.103	2.565	-56.312	-47.528	20.774
600	12.996	21.589	15.159	3.858	-56.088	-45.793	16.680
700	13.077	23.599	16.225	5.162	-55.902	-44.095	13.767
700	13.077	23.599	16.225	5.162	-56.010	-44.095	13.767
800	13.134	25.349	17.259	6.472	-55.850	-42.402	11.583
900	13.213	26.900	18.246	7.789	-55.740	-40.729	9.890
1000	13.338	28.298	19.182	9.116	-55.681	-39.074	8.540
1100	13.521	29.577	20.069	10.459	-55.674	-37.406	7.432
1200	13.765	30.764	20.912	11.823	-55.726	-35.746	6.510
1300	14.066	31.877	21.712	13.214	-55.854	-34.079	5.729
1394	14.394	32.870	22.432	14.551	-56.089	-32.506	5.096
1400	14.415	32.932	22.477	14.637	-56.097	-32.403	5.058
1500	14.804	33.940	23.208	16.098	-56.062	-30.717	4.475
1600	15.220	34.908	23.909	17.599	-55.929	-29.031	3.965
1700	15.649	35.844	24.583	19.143	-55.734	-27.356	3.517
1768	15.941	36.464	25.029	20.217	-55.576	-26.231	3.242
1768	15.941	36.464	25.029	20.217	-59.276	-26.231	3.242
1800	16.078	36.751	25.235	20.729	-59.275	-25.631	3.112

Phase changes: 700 K, α - β transition point of Co; $\Delta H° = 0.108$ kcal/mol.
1394 K, Curie temperature of Co; $\Delta H° \approx 0$ kcal/mol.
1768 K, melting point of Co; $\Delta H° = 3.700$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 10.817 + 2.556\times10^{-3}T + 1.441\times10^{5}T^{-2}$

$H°- H°_{298} = 10.817\times10^{-3}T + 1.278\times10^{-6}T^{2} - 1.441\times10^{2}T^{-1} - 2.855$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf° = -56.861 + 2.201\times10^{-3}T - 0.751\times10^{-6}T^{2} - 178.300T^{-1}$

$\Delta Gf° = -56.861 - 2.201\times10^{-3}T\ln T + 0.751\times10^{-6}T^{2} - 89.150T^{-1} + 32.313\times10^{-3}T$

700-1394 K: $\Delta Hf° = -63.393 + 10.687\times10^{-3}T - 4.389\times10^{-6}T^{2} + 1408.100T^{-1}$

$\Delta Gf° = -63.393 - 10.687\times10^{-3}T\ln T + 4.389\times10^{-6}T^{2} + 704.050T^{-1} + 93.072\times10^{-3}T$

1394-1768 K: $\Delta Hf° = -50.915 - 7.223\times10^{-3}T + 2.619\times10^{-6}T^{2} - 166.700T^{-1}$

$\Delta Gf° = -50.915 + 7.223\times10^{-3}T\ln T - 2.619\times10^{-6}T^{2} - 83.350T^{-1} - 35.372\times10^{-3}T$

1768-1800 K: $\Delta Hf° = -54.779 - 4.314\times10^{-3}T + 1.026\times10^{-6}T^{2} - 166.700T^{-1}$

$\Delta Gf° = -54.779 + 4.314\times10^{-3}T\ln T - 1.026\times10^{-6}T^{2} - 83.350T^{-1} - 14.251\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). Low-temperature heat capacities and entropy at 298 K from King (127). High-temperature data based on King (131).

$Co_3O_4(c)$

Tricobalt Tetraoxide

[Formation: $3Co(c) + 2O_2(g) = Co_3O_4(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	29.480	26.130	26.130	0	-219.600	-191.747	140.552
300	29.593	26.313	26.130	.055	-219.604	-191.571	139.557
400	34.208	35.511	27.354	3.263	-219.658	-182.226	99.563
500	37.008	43.469	29.799	6.835	-219.513	-172.866	75.559
600	38.927	50.394	32.667	10.636	-219.298	-163.558	59.575
700	40.743	56.527	35.646	14.617	-219.057	-154.294	48.172
700	40.743	56.527	35.646	14.617	-219.381	-154.294	48.172
800	43.176	62.116	38.610	18.805	-219.045	-145.010	39.614
900	46.919	67.401	41.517	23.296	-218.582	-135.785	32.973
1000*	52.659	72.621	44.366	28.255	-217.839	-126.650	27.679

*Co_3O_4 decomposes near 1200 K.

Phase change: 700 K, α - β transition point of Co; $\Delta H° = 0.108$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 31.464 + 15.778\times10^{-3}T - 5.928\times10^{5}T^{-2}$

$H°- H°_{298} = 31.464\times10^{-3}T + 7.889\times10^{-6}T^{2} + 5.928\times10^{2}T^{-1} - 12.071$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf° = -221.903 + 2.001\times10^{-3}T + 1.552\times10^{-6}T^{2} + 467.600T^{-1}$

$\Delta Gf° = -221.903 - 2.001\times10^{-3}T\ln T - 1.552\times10^{-6}T^{2} + 233.800T^{-1} + 110.378\times10^{-3}T$

700-1000 K: $\Delta Hf° = -241.499 + 27.459\times10^{-3}T - 9.362\times10^{-6}T^{2} + 5226.800T^{-1}$

$\Delta Gf° = -241.499 - 27.459\times10^{-3}T\ln T + 9.362\times10^{-6}T^{2} + 2613.400T^{-1} + 292.653\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Sreedharan (211). Low-temperature heat capacities from King (127) and Khriplovich (125), whose entropy at 298 K was used. High-temperature data based on King (131).

Cr(c,1)

Chromium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.580	5.650	5.650	0
300	5.590	5.680	5.650	.010
311.5	7.620	5.900	5.653	.077
400	6.020	7.350	5.872	.591
500	6.410	8.740	6.314	1.213
600	6.730	9.940	6.822	1.871
700	7.000	11.000	7.346	2.558
800	7.220	11.950	7.862	3.270
900	7.420	12.810	8.366	4.000
1000	7.660	13.600	8.848	4.752
1100	8.050	14.350	9.315	5.538
1200	8.480	15.070	9.768	6.362
1300	8.890	15.760	10.196	7.233
1400	9.270	16.430	10.614	8.142
1500	9.680	17.090	11.031	9.088
1600	10.140	17.730	11.430	10.080
1700	10.540	18.350	11.812	11.114
1800	10.920	18.970	12.199	12.188
1900	11.270	19.570	12.568	13.303
2000	11.650	20.160	12.936	14.449
2100	11.990	20.740	13.296	15.632
2130	12.100	20.910	13.402	15.993
2130	9.400	22.810	13.402	20.040
2200	9.400	23.110	13.702	20.698
2300	9.400	23.530	14.122	21.638
2400	9.400	23.930	14.523	22.578
2500	9.400	24.320	14.913	23.518

Phase changes: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
2130 K, melting point of Cr; ΔH° = 4.047 kcal/mol.
2945 K, boiling point of Cr; ΔH° = 82.3 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-311.5 K: $Cp^\circ = -2.808 + 28.134\times10^{-3}T$

$H^\circ - H^\circ_{298} = -2.808\times10^{-3}T + 14.067\times10^{-6}T^2 - 0.413$

311.5-2130 K: $Cp^\circ = 4.359 + 3.582\times10^{-3}T + 0.136\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.359\times10^{-3}T + 1.791\times10^{-6}T^2 - 0.136\times10^{2}T^{-1} - 1.411$

2130-2500 K: $Cp^\circ = 9.400$

$H^\circ - H^\circ_{298} = 9.400\times10^{-3}T + 0.018$

Sources: Data for the transition at 311.5 K from the heat capacity measurements (200 to 380 K) of Williams (252). All other data from Hultgren (99).

Cr(g)

Chromium (ideal monatomic gas)

[Formation: Cr(c,1) = Cr(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	41.635	41.635	0	95.000	84.271	-61.772
300	4.968	41.665	41.635	.009	94.999	84.204	-61.341
311.5	4.968	41.852	41.640	.066	94.989	83.790	-58.787
400	4.968	43.094	41.829	.506	94.915	80.617	-44.047
500	4.968	44.203	42.197	1.003	94.790	77.059	-33.682
600	4.968	45.109	42.609	1.500	94.629	73.528	-26.782
700	4.968	45.875	43.024	1.996	94.438	70.026	-21.863
800	4.969	46.538	43.422	2.493	94.223	66.553	-18.181
900	4.972	47.123	43.801	2.990	93.990	63.108	-15.325
1000	4.980	47.648	44.160	3.488	93.736	59.688	-13.045
1100	4.995	48.123	44.499	3.986	93.448	56.298	-11.185
1200	5.023	48.559	44.820	4.487	93.125	52.938	-9.641
1300	5.065	48.962	45.123	4.991	92.758	49.595	-8.338
1400	5.124	49.340	45.411	5.501	92.359	46.285	-7.225
1500	5.203	49.696	45.685	6.017	91.929	43.020	-6.268
1600	5.299	50.034	45.945	6.542	91.462	39.776	-5.433
1700	5.414	50.359	46.196	7.077	90.963	36.548	-4.698
1800	5.544	50.672	46.436	7.625	90.437	33.373	-4.052
1900	5.688	50.976	46.667	8.187	89.884	30.213	-3.475
2000	5.841	51.271	46.889	8.763	89.314	27.092	-2.960
2100	6.001	51.560	47.105	9.355	88.723	24.001	-2.498
2130	6.050	51.645	47.169	9.536	88.543	23.076	-2.368
2130	6.050	51.645	47.169	9.536	84.496	23.076	-2.368
2200	6.165	51.843	47.314	9.963	84.265	21.052	-2.091
2300	6.329	52.121	47.518	10.588	83.950	18.191	-1.728
2400	6.492	52.394	47.715	11.229	83.651	15.337	-1.397
2500	6.651	52.662	47.908	11.886	83.368	12.513	-1.094

Phase changes: 311.5 K, second-order transition point of Cr; $\Delta H° = 0$ kcal/mol.
2130 K, melting point of Cr; $\Delta H° = 4.047$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 4.433 + 0.606\times10^{-3}T + 0.315\times10^{5}T^{-2}$

$H°- H°_{298} = 4.433\times10^{-3}T + 0.303\times10^{-6}T^{2} - 0.315\times10^{2}T^{-1} - 1.243$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = 94.170 + 7.241\times10^{-3}T - 13.764\times10^{-6}T^{2} - 31.500T^{-1}$

$\Delta Gf° = 94.170 - 7.241\times10^{-3}T\ln T + 13.764\times10^{-6}T^{2} - 15.750T^{-1} + 4.128\times10^{-3}T$

311.5-2130 K: $\Delta Hf° = 95.168 + 0.074\times10^{-3}T - 1.488\times10^{-6}T^{2} - 17.900T^{-1}$

$\Delta Gf° = 95.168 - 0.074\times10^{-3}T\ln T + 1.488\times10^{-6}T^{2} - 8.950T^{-1} - 36.470\times10^{-3}T$

2130-2500 K: $\Delta Hf° = 93.739 - 4.967\times10^{-3}T + 0.303\times10^{-6}T^{2} - 31.500T^{-1}$

$\Delta Gf° = 93.739 + 4.967\times10^{-3}T\ln T - 0.303\times10^{-6}T^{2} - 15.750T^{-1} - 70.616\times10^{-3}T$

Source: Data from Chase (33).

CrO(g)

Chromium Oxide (ideal gas)

[Formation: $Cr(c,1) + 0.5O_2(g) = CrO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.486	57.159	57.159	0	45.000	36.948	-27.083
300	7.494	57.206	57.159	.014	44.998	36.897	-26.879
311.5	7.539	57.489	57.166	.100	44.976	36.587	-25.669
400	7.883	59.417	57.459	.783	44.831	34.222	-18.698
500	8.174	61.209	58.035	1.587	44.647	31.593	-13.809
600	8.380	62.718	58.693	2.415	44.440	29.002	-10.564
700	8.527	64.022	59.363	3.261	44.210	26.448	-8.257
800	8.634	65.168	60.019	4.119	43.957	23.926	-6.536
900	8.715	66.190	60.649	4.987	43.688	21.439	-5.206
1000	8.777	67.111	61.249	5.862	43.397	18.981	-4.148
1100	8.827	67.950	61.821	6.742	43.072	16.556	-3.289
1200	8.868	68.720	62.364	7.627	42.708	14.165	-2.580
1300	8.903	69.431	62.881	8.515	42.298	11.794	-1.983
1400	8.932	70.092	63.373	9.407	41.849	9.459	-1.477
1500	8.958	70.709	63.841	10.302	41.363	7.174	-1.045
1600	8.981	71.288	64.289	11.199	40.829	4.911	-.671
1700	9.001	71.833	64.717	12.098	40.253	2.673	-.344
1800	9.020	72.348	65.126	12.999	39.636	.491	-.060
1900	9.038	72.837	65.520	13.902	38.977	-1.673	.192
2000	9.055	73.301	65.897	14.807	38.286	-3.790	.414
2100	9.071	73.743	66.261	15.713	37.557	-5.869	.611
2130	9.076	73.872	66.367	15.985	37.332	-6.489	.666
2130	9.076	73.872	66.367	15.985	33.285	-6.489	.666
2200	9.087	74.165	66.610	16.621	32.944	-7.799	.775
2300	9.103	74.569	66.947	17.530	32.455	-9.635	.916
2400	9.119	74.957	67.273	18.441	31.966	-11.455	1.043
2500	9.135	75.330	67.588	19.354	31.476	-13.240	1.157

*All data except enthalpy of formation at 298 K estimated.

Phase changes: 311.5 K, second-order transition point of Cr; $\Delta H° = 0$ kcal/mol.
2130 K, melting point of Cr; $\Delta H° = 4.047$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 8.466 + 0.336\times10^{-3}T - 0.960\times10^{5}T^{-2}$

$H°- H°_{298} = 8.466\times10^{-3}T + 0.168\times10^{-6}T^{2} + 0.960\times10^{2}T^{-1} - 2.861$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = 43.728 + 7.659\times10^{-3}T - 14.150\times10^{-6}T^{2} + 73.400T^{-1}$

$\Delta Gf° = 43.728 - 7.659\times10^{-3}T\ln T + 14.150\times10^{-6}T^{2} + 36.700T^{-1} + 16.265\times10^{-3}T$

311.5-2000 K: $\Delta Hf° = 44.726 + 0.492\times10^{-3}T - 1.874\times10^{-6}T^{2} + 87.000T^{-1}$

$\Delta Gf° = 44.726 - 0.492\times10^{-3}T\ln T + 1.874\times10^{-6}T^{2} + 43.500T^{-1} - 24.332\times10^{-3}T$

2000-2130 K: $\Delta Hf° = 45.394 - 0.063\times10^{-3}T - 1.728\times10^{-6}T^{2} - 205.400T^{-1}$

$\Delta Gf° = 45.394 + 0.063\times10^{-3}T\ln T + 1.728\times10^{-6}T^{2} - 102.700T^{-1} - 28.554\times10^{-3}T$

2130-2500 K: $\Delta Hf° = 43.965 - 5.104\times10^{-3}T + 0.063\times10^{-6}T^{2} - 219.000T^{-1}$

$\Delta Gf° = 43.965 + 5.104\times10^{-3}T\ln T - 0.063\times10^{-6}T^{2} - 109.500T^{-1} - 62.701\times10^{-3}T$

Source: Data from Chase (33) who estimated all except enghalpy of formation at 298 K.

$CrO_2(g)$

Chromium Dioxide (ideal gas)

[Formation: $Cr(c,l) + O_2(g) = CrO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	10.370	64.323	64.323	0	-18.000	-20.883	15.307
300	10.387	64.387	64.324	.019	-18.004	-20.901	15.226
311.5	10.485	64.780	64.333	.139	-18.032	-21.012	14.742
400	11.236	67.496	64.741	1.102	-18.212	-21.834	11.930
500	11.889	70.077	65.557	2.260	-18.407	-22.715	9.929
600	12.359	72.288	66.500	3.473	-18.607	-23.558	8.581
700	12.696	74.220	67.467	4.727	-18.818	-24.365	7.607
800	12.940	75.932	68.421	6.009	-19.046	-25.144	6.869
900	13.120	77.467	69.341	7.313	-19.286	-25.890	6.287
1000	13.256	78.857	70.225	8.632	-19.546	-26.613	5.816
1100	13.361	80.126	71.069	9.963	-19.840	-27.305	5.425
1200	13.443	81.292	71.873	11.303	-20.172	-27.965	5.093
1300	13.508	82.370	72.638	12.651	-20.551	-28.607	4.809
1400	13.561	83.373	73.369	14.005	-20.970	-29.216	4.561
1500	13.604	84.311	74.069	15.363	-21.428	-29.780	4.339
1600	13.639	85.190	74.737	16.725	-21.935	-30.321	4.142
1700	13.669	86.017	75.375	18.091	-22.485	-30.837	3.964
1800	13.694	86.800	75.989	19.459	-23.079	-31.301	3.800
1900	13.716	87.541	76.578	20.829	-23.718	-31.747	3.652
2000	13.734	88.245	77.144	22.202	-24.390	-32.148	3.513
2100	13.750	88.915	77.688	23.576	-25.104	-32.511	3.383
2130	13.754	89.110	77.848	23.989	-25.325	-32.616	3.347
2130	13.754	89.110	77.848	23.989	-29.372	-32.616	3.347
2200	13.764	89.555	78.213	24.952	-29.704	-32.727	3.251
2300	13.776	90.167	78.720	26.329	-30.183	-32.849	3.121
2400	13.787	90.754	79.209	27.707	-30.666	-32.956	3.001
2500	13.797	91.317	79.683	29.086	-31.153	-33.026	2.887

*All data except enthalpy of formation at 298 K estimated.

Phase changes: 311.5 K, second-order transition point of Cr; ΔH° = 0 kcal/mol.
2130 K, melting point of Cr; ΔH° = 4.047 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp^\circ = 12.631 + 0.658\times10^{-3}T - 2.184\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 12.631\times10^{-3}T + 0.329\times10^{-6}T^2 + 2.184\times10^{2}T^{-1} - 4.528$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = -19.762 + 8.209\times10^{-3}T - 14.241\times10^{-6}T^2 + 173.200T^{-1}$

$\Delta Gf^\circ = -19.762 - 8.209\times10^{-3}T\ln T + 14.241\times10^{-6}T^2 + 86.600T^{-1} + 37.795\times10^{-3}T$

311.5-2000 K: $\Delta Hf^\circ = -18.765 + 1.042\times10^{-3}T - 1.965\times10^{-6}T^2 + 186.800T^{-1}$

$\Delta Gf^\circ = -18.765 - 1.042\times10^{-3}T\ln T + 1.965\times10^{-6}T^2 + 93.400T^{-1} - 2.803\times10^{-3}T$

2000-2130 K: $\Delta Hf^\circ = -17.428 - 0.068\times10^{-3}T - 1.671\times10^{-6}T^2 - 398.000T^{-1}$

$\Delta Gf^\circ = -17.428 + 0.068\times10^{-3}T\ln T + 1.671\times10^{-6}T^2 - 199.000T^{-1} - 11.247\times10^{-3}T$

2130-2500 K: $\Delta Hf^\circ = -18.857 - 5.109\times10^{-3}T + 0.120\times10^{-6}T^2 - 411.600T^{-1}$

$\Delta Gf^\circ = -18.857 + 5.109\times10^{-3}T\ln T - 0.120\times10^{-6}T^2 - 205.800T^{-1} - 45.393\times10^{-3}T$

Source: Data from Chase (33) who estimated all except enthalpy of formation at 298 K.

$CrO_3(g)$

Chromium Trioxide (ideal gas)

[Formation: $Cr(c,1) + 1.5O_2(g) = CrO_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.390	63.591	63.591	0	-70.000	-65.359	47.909
300	13.430	63.674	63.591	.025	-70.005	-65.331	47.593
311.5	13.640	64.183	63.603	.181	-70.037	-65.151	45.709
400	15.258	67.804	64.142	1.465	-70.211	-63.738	34.824
500	16.500	71.351	65.237	3.057	-70.337	-62.102	27.144
600	17.338	74.438	66.520	4.751	-70.434	-60.445	22.017
700	17.914	77.157	67.848	6.516	-70.522	-58.772	18.349
800	18.321	79.577	69.166	8.329	-70.618	-57.088	15.596
900	18.617	81.753	70.446	10.176	-70.723	-55.391	13.450
1000	18.838	83.726	71.676	12.050	-70.841	-53.682	11.732
1100	19.006	85.530	72.855	13.942	-70.993	-51.958	10.323
1200	19.137	87.190	73.982	15.850	-71.182	-50.215	9.145
1300	19.241	88.726	75.058	17.769	-71.418	-48.468	8.148
1400	19.324	90.155	76.086	19.697	-71.695	-46.698	7.290
1500	19.393	91.491	77.069	21.633	-72.010	-44.992	6.541
1600	19.449	92.744	78.010	23.575	-72.375	-43.072	5.883
1700	19.496	93.924	78.911	25.522	-72.785	-41.238	5.301
1800	19.535	95.040	79.777	27.474	-73.239	-39.358	4.779
1900	19.569	96.097	80.608	29.429	-73.740	-37.468	4.310
2000	19.598	97.102	81.408	31.388	-74.276	-35.541	3.884
2100	19.623	98.058	82.178	33.349	-74.855	-33.582	3.495
2130	19.630	98.336	82.403	33.938	-75.036	-32.992	3.385
2130	19.630	98.336	82.403	33.938	-79.083	-32.992	3.385
2200	19.645	98.972	82.921	35.312	-79.323	-31.485	3.128
2300	19.664	99.846	83.638	37.278	-79.671	-29.299	2.784
2400	19.681	100.683	84.331	39.245	-80.026	-27.101	2.468
2500	19.695	101.486	85.000	41.214	-80.386	-24.871	2.174

*All data except enthalpy of formation at 298 K estimated.

Phase changes: 311.5 K, second-order transition point of Cr; $\Delta H° = 0$ kcal/mol.
2130 K, melting point of Cr; $\Delta H° = 4.047$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 18.095 + 0.918\times10^{-3}T - 4.425\times10^{5}T^{-2}$

$H°- H°_{298} = 18.095\times10^{-3}T + 0.459\times10^{-6}T^{2} + 4.425\times10^{2}T^{-1} - 6.920$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = -72.979 + 10.058\times10^{-3}T - 14.363\times10^{-6}T^{2} + 374.700T^{-1}$

$\Delta Gf° = -72.979 - 10.058\times10^{-3}T\ln T + 14.363\times10^{-6}T^{2} + 187.350T^{-1} + 76.474\times10^{-3}T$

311.5-2000 K: $\Delta Hf° = -71.981 + 2.891\times10^{-3}T - 2.087\times10^{-6}T^{2} + 388.300T^{-1}$

$\Delta Gf° = -71.981 - 2.891\times10^{-3}T\ln T + 2.087\times10^{-6}T^{2} + 194.150T^{-1} + 35.877\times10^{-3}T$

2000-2130 K: $\Delta Hf° = -69.977 + 1.226\times10^{-3}T - 1.645\times10^{-6}T^{2} - 488.900T^{-1}$

$\Delta Gf° = -69.977 - 1.226\times10^{-3}T\ln T + 1.645\times10^{-6}T^{2} - 244.450T^{-1} + 23.210\times10^{-3}T$

2130-2500 K: $\Delta Hf° = -71.405 - 3.815\times10^{-3}T + 0.145\times10^{-6}T^{2} - 502.500T^{-1}$

$\Delta Gf° = -71.405 + 3.815\times10^{-3}T\ln T - 0.145\times10^{-6}T^{2} - 251.250T^{-1} - 10.936\times10^{-3}T$

Source: Data from Chase (33) who estimated all except enthalpy of formation at 298 K.

$Cr_2O_3(c)$

Dichromium Trioxide

[Formation: $2Cr(c) + 1.5O_2(g) = Cr_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	28.680	19.400	19.400	0	-272.600	-253.099	185.524
300	29.030	19.580	19.403	.053	-272.586	-252.980	184.294
305	30.500	20.070	19.408	.202	-272.551	-252.653	181.038
311.5	30.242	20.710	19.428	.399	-272.495	-252.229	176.963
400	26.730	27.280	20.455	2.730	-272.137	-246.515	134.688
500	28.110	33.440	22.460	5.490	-271.717	-240.156	104.971
600	28.740	38.620	24.720	8.340	-271.316	-233.872	85.187
700	29.230	43.090	27.033	11.240	-270.957	-227.659	71.077
800	29.730	47.030	29.299	14.185	-270.633	-221.505	60.511
900	30.200	50.550	31.456	17.185	-270.314	-215.370	52.298
1000	30.600	53.760	33.535	20.225	-270.018	-209.293	45.740
1100	30.920	56.690	35.508	23.300	-269.773	-203.229	40.377
1200	31.140	59.390	37.386	26.405	-269.589	-197.178	35.911
1300	31.270	61.890	39.178	29.525	-269.495	-191.170	32.138
1400	31.330	64.210	40.885	32.655	-269.479	-185.157	28.904
1500	31.340	66.370	42.510	35.790	-269.541	-179.106	26.095
1600	31.340	68.390	44.062	38.925	-269.705	-173.067	23.640
1700	31.350	70.290	45.549	42.060	-269.961	-167.041	21.474
1800	31.410	72.090	46.982	45.195	-270.306	-160.969	19.544
1900	31.560	73.790	48.345	48.345	-270.727	-154.889	17.816
2000	31.830	75.410	49.655	51.510	-271.203	-148.764	16.256

Phase changes: 305 K, second order transition point of Cr_2O_3; $\Delta H° = 0$ kcal/mol.
311.5 K, second order transition point of Cr; $\Delta H° = 0$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-305 K:

$$Cp° = 29.489$$

$$H°- H°_{298} = 29.489\times10^{-3}T - 8.792$$

305-2000 K:

$$Cp° = 26.207 + 3.694\times10^{-3}T$$

$$H°- H°_{298} = 26.207\times10^{-3}T + 1.847\times10^{-6}T^2 - 7.963$$

Formation equations (kcal/mol):

298.15-305 K:

$$\Delta Hf° = -277.038 + 24.260\times10^{-3}T - 28.889\times10^{-6}T^2 - 67.800T^{-1}$$

$$\Delta Gf° = -277.038 - 24.260\times10^{-3}T\ln T + 28.889\times10^{-6}T^2 - 33.900T^{-1} + 210.284\times10^{-3}T$$

305-311.5 K:

$$\Delta Hf° = -276.209 + 20.978\times10^{-3}T - 27.042\times10^{-6}T^2 - 67.800T^{-1}$$

$$\Delta Gf° = -276.209 - 20.978\times10^{-3}T\ln T + 27.042\times10^{-6}T^2 - 33.900T^{-1} + 189.354\times10^{-3}T$$

311.5-2000 K:

$$\Delta Hf° = -274.213 + 6.644\times10^{-3}T - 2.490\times10^{-6}T^2 - 40.600T^{-1}$$

$$\Delta Gf° = -274.213 - 6.644\times10^{-3}T\ln T + 2.490\times10^{-6}T^2 - 20.300T^{-1} + 108.159\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Mah (147). Low-temperature heat capacities and entropy at 298 K from Anderson (7). High-temperature data based on Kelley (120).

Cs(c,1,g)

Cesium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	7.695	20.370	20.370	0
300	7.733	20.418	20.371	.014
301.55	7.747	20.458	20.372	.026
301.55	7.744	22.116	20.372	.526
400	7.533	24.268	21.078	1.276
500	7.446	25.939	21.889	2.025
600	7.409	27.293	22.681	2.767
700	7.395	28.434	23.424	3.507
800	7.393	29.421	24.112	4.247
900	7.399	30.292	24.752	4.986
952	7.404	30.695	25.053	5.371
952	4.968	47.710	25.053	21.569
1000	4.968	47.954	26.147	21.807
1100	4.968	48.428	28.152	22.304
1200	4.969	48.860	29.860	22.800
1300	4.971	49.258	31.337	23.297
1400	4.975	49.627	32.631	23.795
1500	4.981	49.970	33.775	24.292
1600	4.992	50.292	34.798	24.791
1700	5.008	50.595	35.718	25.291
1800	5.031	50.882	36.553	25.793
1900	5.062	51.154	37.313	26.297
2000	5.102	51.415	38.013	26.805

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
952 K, calculated boiling point to ideal monatomic gas; ΔH° = 16.198 kcal/mol.
941 K, normal boiling point to equilbrium mixture of Cs(g) and Cs_2(g).

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-301.55 K: $C_p^\circ = 3.136 + 15.294\times10^{-3}T$

$H^\circ - H^\circ_{298} = 3.136\times10^{-3}T + 7.647\times10^{-6}T^2 - 1.615$

301.55-952 K: $C_p^\circ = 7.133 + 0.230\times10^{-3}T + 0.493\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.133\times10^{-3}T + 0.115\times10^{-6}T^2 - 0.493\times10^{2}T^{-1} - 1.472$

952-2000 K: $C_p^\circ = 4.759 + 0.128\times10^{-3}T + 0.789\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.759\times10^{-3}T + 0.064\times10^{-6}T^2 - 0.789\times10^{2}T^{-1} + 17.063$

Sources: Entropy at 298 K from CODATA (36). All other data from JANAF (51).

Cs(g)

Cesium (ideal monatomic gas)

[Formation: Cs(c,1,g) = Cs(g)]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	41.942	41.942	0	18.320	11.888	-8.714
300	4.968	41.973	41.943	.009	18.315	11.849	-8.632
301.55	4.968	41.999	41.943	.017	18.311	11.815	-8.563
301.55	4.968	41.999	41.943	.017	17.811	11.815	-8.563
400	4.968	43.402	42.137	.506	17.550	9.896	-5.407
500	4.968	44.511	42.505	1.003	17.298	8.012	-3.502
600	4.968	45.417	42.917	1.500	17.053	6.179	-2.251
700	4.968	46.182	43.331	1.996	16.809	4.385	-1.369
800	4.968	46.846	43.730	2.493	16.566	2.626	-.717
900	4.968	47.431	44.109	2.990	16.324	.899	-.218
952	4.968	47.710	44.297	3.249	16.198	0	0
952	4.968	47.710	44.297	3.249	0	0	0
1000	4.968	47.954	44.467	3.487	0	0	0
1100	4.968	48.428	44.806	3.984	0	0	0
1200	4.969	48.860	45.127	4.480	0	0	0
1300	4.971	49.258	45.430	4.977	0	0	0
1400	4.975	49.627	45.716	5.475	0	0	0
1500	4.981	49.970	45.989	5.972	0	0	0
1600	4.992	50.292	46.248	6.471	0	0	0
1700	5.008	50.595	46.494	6.971	0	0	0
1800	5.031	50.882	46.730	7.473	0	0	0
1900	5.062	51.154	46.956	7.977	0	0	0
2000	5.102	51.415	47.173	8.485	0	0	0

Phase changes: 301.55 K, melting point of Cs; $\Delta H° = 0.500$ kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; $\Delta H° = 16.198$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.947 + 0.028\times10^{-3}T + 0.011\times10^{5}T^{-2}$

$H°- H°_{298} = 4.947\times10^{-3}T + 0.014\times10^{-6}T^{2} - 0.011\times10^{2}T^{-1} - 1.473$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = 18.462 + 1.811\times10^{-3}T - 7.633\times10^{-6}T^{2} - 1.100T^{-1}$

$\Delta Gf° = 18.462 - 1.811\times10^{-3}T\ln T + 7.633\times10^{-6}T^{2} - 0.550T^{-1} - 14.000\times10^{-3}T$

301.55-952 K: $\Delta Hf° = 18.319 - 2.186\times10^{-3}T - 0.101\times10^{-6}T^{2} + 48.200T^{-1}$

$\Delta Gf° = 18.319 + 2.186\times10^{-3}T\ln T + 0.101\times10^{-6}T^{2} + 24.100T^{-1} - 34.344\times10^{-3}T$

952-2000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Source: Data from JANAF (51).

$Cs_2(g)$

Cesium (ideal diatomic gas)

[Formation: $2Cs(c,l,g) = Cs_2(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.114	68.053	68.053	0	25.400	17.257	-12.649
300	9.115	68.108	68.051	.017	25.389	17.207	-12.535
301.55	9.116	68.155	68.052	.031	25.379	17.165	-12.440
301.55	9.116	68.155	68.052	.031	24.379	17.165	-12.440
400	9.178	70.739	68.411	.931	23.779	14.898	-8.140
500	9.240	72.794	69.090	1.852	23.202	12.744	-5.570
600	9.300	74.484	69.852	2.779	22.645	10.706	-3.900
700	9.361	75.922	70.619	3.712	22.098	8.760	-2.735
800	9.421	77.176	71.362	4.651	21.557	6.890	-1.882
900	9.481	78.289	72.071	5.596	21.024	5.089	-1.236
952	9.513	78.822	72.425	6.091	20.749	4.153	-.953
952	9.513	78.822	72.425	6.091	-11.647	4.153	-.953
1000	9.542	79.291	72.743	6.548	-11.666	4.951	-1.082
1100	9.604	80.203	73.380	7.505	-11.703	6.615	-1.314
1200	9.666	81.042	73.985	8.468	-11.732	8.282	-1.508
1300	9.731	81.818	74.558	9.438	-11.756	9.951	-1.673
1400	9.799	82.542	75.103	10.415	-11.775	11.622	-1.814
1500	9.871	83.220	75.621	11.398	-11.786	13.294	-1.937
1600	9.946	83.859	76.116	12.389	-11.793	14.967	-2.044
1700	10.027	84.465	76.590	13.388	-11.794	16.639	-2.139
1800	10.114	85.040	77.043	14.395	-11.791	18.312	-2.223
1900	10.207	85.590	77.479	15.411	-11.783	19.981	-2.298
2000	10.306	86.116	77.898	16.436	-11.774	21.654	-2.366

Phase changes: 301.55 K, melting point of Cs; $\Delta H° = 0.500$ kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; $\Delta H° = 16.198$ kcal/mol of Cs.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.900 + 0.652\times10^{-3}T + 0.017\times10^{5}T^{-2}$

$H°- H°_{298} = 8.900\times10^{-3}T + 0.326\times10^{-6}T^2 - 0.017\times10^{2}T^{-1} - 2.677$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = 25.953 + 2.628\times10^{-3}T - 14.968\times10^{-6}T^2 - 1.700T^{-1}$

$\Delta Gf° = 25.953 - 2.628\times10^{-3}T\ln T + 14.968\times10^{-6}T^2 - 0.850T^{-1} - 18.647\times10^{-3}T$

301.55-952 K: $\Delta Hf° = 25.667 - 5.366\times10^{-3}T + 0.096\times10^{-6}T^2 + 96.900T^{-1}$

$\Delta Gf° = 25.667 + 5.366\times10^{-3}T\ln T - 0.096\times10^{-6}T^2 + 48.450T^{-1} - 59.334\times10^{-3}T$

952-2000 K: $\Delta Hf° = -11.404 - 0.618\times10^{-3}T + 0.198\times10^{-6}T^2 + 156.100T^{-1}$

$\Delta Gf° = -11.404 + 0.618\times10^{-3}T\ln T - 0.198\times10^{-6}T^2 + 78.050T^{-1} + 12.234\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from JANAF (51). All other data from Behrens (15).

CsO(g)

Cesium Oxide (ideal gas)

[Formation: $Cs(c,l,g) + 0.5O_2(g) = CsO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.719	61.049	61.049	0	15.000	10.177	-7.460
300	8.722	61.103	61.050	.016	14.995	10.147	-7.392
301.55	8.724	61.148	61.050	.030	14.992	10.122	-7.336
301.55	8.724	61.148	61.050	.030	14.492	10.122	-7.336
400	8.854	63.632	61.392	.896	14.259	8.731	-4.770
500	8.927	65.616	62.046	1.785	14.033	7.375	-3.223
600	8.976	67.249	62.782	2.680	13.809	6.064	-2.209
700	9.013	68.635	63.521	3.580	13.580	4.792	-1.496
800	9.043	69.841	64.237	4.483	13.344	3.551	-.970
900	9.069	70.907	64.920	5.388	13.103	2.343	-.569
952	9.081	71.417	65.262	5.860	12.975	1.712	-.393
952	9.081	71.417	65.262	5.860	-3.223	1.712	-.393
1000	9.093	71.864	65.568	6.296	-3.224	1.961	-.429
1100	9.115	72.732	66.180	7.207	-3.229	2.481	-.493
1200	9.137	73.526	66.760	8.119	-3.237	3.000	-.546
1300	9.157	74.258	67.309	9.034	-3.248	3.521	-.592
1400	9.177	74.937	67.829	9.951	-3.260	4.043	-.631
1500	9.196	75.571	68.325	10.869	-3.274	4.564	-.665
1600	9.216	76.165	68.796	11.790	-3.291	5.087	-.695
1700	9.235	76.724	69.246	12.712	-3.310	5.612	-.721
1800	9.253	77.253	69.677	13.637	-3.331	6.137	-.745
1900	9.272	77.753	70.088	14.563	-3.356	6.664	-.766
2000	9.290	78.230	70.485	15.491	-3.385	7.191	-.786

*All data estimated.

Phase changes: 301.55 K, melting point of Cs; $\Delta H° = 0.500$ kcal/mol.
952 K, boiling point of Cs to ideal gas; $\Delta H° = 16.198$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.929 + 0.186\times10^{-3}T - 0.236\times10^{5}T^{-2}$

$H°- H°_{298} = 8.929\times10^{-3}T + 0.093\times10^{-6}T^{2} + 0.236\times10^{2}T^{-1} - 2.750$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = 15.041 + 2.178\times10^{-3}T - 7.805\times10^{-6}T^{2} + 1.000T^{-1}$

$\Delta Gf° = 15.041 - 2.178\times10^{-3}T\ln T + 7.805\times10^{-6}T^{2} + 0.500T^{-1} - 6.238\times10^{-3}T$

301.55-952 K: $\Delta Hf° = 14.898 - 1.819\times10^{-3}T - 0.273\times10^{-6}T^{2} + 50.300T^{-1}$

$\Delta Gf° = 14.898 + 1.819\times10^{-3}T\ln T + 0.273\times10^{-6}T^{2} + 25.150T^{-1} - 26.582\times10^{-3}T$

952-2000 K: $\Delta Hf° = -3.637 + 0.555\times10^{-3}T - 0.222\times10^{-6}T^{2} + 79.900T^{-1}$

$\Delta Gf° = -3.637 - 0.555\times10^{-3}T\ln T + 0.222\times10^{-6}T^{2} + 39.950T^{-1} + 9.203\times10^{-3}T$

Source: Data are those estimated by JANAF (51).

$Cs_2O(c)$

Dicesium Oxide

[Formation: $2Cs(c,l) + 0.5O_2(g) = Cs_2O(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.160	35.100	35.100	0	-82.690	-73.703	54.025
300	18.180	35.220	35.107	.034	-82.691	-73.648	53.652
301.55	18.192	35.314	35.107	.062	-82.692	-73.602	53.342
301.55	18.192	35.314	35.107	.062	-83.692	-73.602	53.342
400*	18.980	40.560	35.835	1.890	-83.714	-70.305	38.412
500	19.790	44.890	37.230	3.830	-83.637	-66.963	29.269
600	20.580	48.540	38.798	5.845	-83.484	-63.627	23.176
700	21.370	51.790	40.440	7.945	-83.253	-60.344	18.840
763	21.890	53.660	41.465	9.305	-83.076	-58.300	16.699

*Data extrapolated 350 to 763 K.

Phase changes: 301.55 K, melting point of Cs; $\Delta H° = 0.500$ kcal/mol.
763 K, melting point of Cs_2O.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-763 K: $Cp° = 15.854 + 7.888\times10^{-3}T - 0.040\times10^{5}T^{-2}$

$H°- H°_{298} = 15.854\times10^{-3}T + 3.944\times10^{-6}T^2 + 0.040\times10^{2}T^{-1} - 5.091$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = -83.375 + 5.967\times10^{-3}T - 11.601\times10^{-6}T^2 - 18.600T^{-1}$

$\Delta Gf° = -83.375 - 5.967\times10^{-3}T\ln T + 11.601\times10^{-6}T^2 - 9.300T^{-1} + 63.084\times10^{-3}T$

301.55-763 K: $\Delta Hf° = -83.662 - 2.027\times10^{-3}T + 3.463\times10^{-6}T^2 + 80.000T^{-1}$

$\Delta Gf° = -83.662 + 2.027\times10^{-3}T\ln T - 3.463\times10^{-6}T^2 + 40.000T^{-1} + 22.397\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Settle (193). Other data from Flotow (66) who extrapolated heat capacities, 350 to 763 K.

$Cs_2O(g)$

Dicesium Oxide (ideal gas)

[Formation: $2Cs(c,l,g) + 0.5O_2(g) = Cs_2O(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.238	75.998	75.998	0	-22.000	-25.207	18.477
300	13.245	76.079	75.999	.024	-22.010	-25.226	18.377
301.55	13.249	76.147	76.000	.045	-22.019	-25.243	18.294
301.55	13.249	76.147	76.000	.045	-23.019	-25.243	18.294
400	13.521	79.933	76.521	1.365	-23.549	-25.889	14.145
500	13.657	82.966	77.518	2.724	-24.053	-26.417	11.547
600	13.732	85.464	78.641	4.094	-24.545	-26.842	9.777
700	13.779	87.584	79.770	5.470	-25.038	-27.185	8.487
800	13.809	89.426	80.865	6.849	-25.538	-27.461	7.502
900	13.830	91.054	81.908	8.231	-26.041	-27.670	6.719
952	13.838	91.831	82.429	8.951	-26.305	-27.780	6.377
952	13.838	91.831	82.429	8.951	-58.701	-27.780	6.377
1000	13.845	92.512	82.897	9.615	-58.712	-26.221	5.731
1100	13.856	93.832	83.832	11.000	-58.741	-22.970	4.564
1200	13.865	95.038	84.716	12.386	-58.771	-19.715	3.591
1300	13.872	96.148	85.553	13.773	-58.806	-16.459	2.767
1400	13.877	97.176	86.347	15.161	-58.846	-13.199	2.060
1500	13.881	98.134	87.102	16.548	-58.888	-9.939	1.448
1600	13.885	99.030	87.819	17.937	-58.935	-6.673	.912
1700	13.888	99.872	88.504	19.325	-58.988	-3.406	.438
1800	13.890	100.666	89.158	20.714	-59.047	-0.135	.016
1900	13.892	101.417	89.784	22.103	-59.113	3.138	-.361
2000	13.894	102.129	90.382	23.493	-59.188	6.420	-.701

*All data except enthalpy of formation at 298 K estimated.

Phase changes: 301.55 K, melting point of Cs; $\Delta H°$ = 0.500 kcal/mol.
952 K, boiling point of Cs to ideal gas; $\Delta H°$ = 16.198 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.878 + 0.020\times10^{-3}T - 0.574\times10^{5}T^{-2}$

$H°- H°_{298} = 13.878\times10^{-3}T + 0.010\times10^{-6}T^2 + 0.574\times10^{2}T^{-1} - 4.331$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = -21.926 + 3.991\times10^{-3}T - 15.535\times10^{-6}T^2 + 34.800T^{-1}$

$\Delta Gf° = -21.926 - 3.991\times10^{-3}T\ln T + 15.535\times10^{-6}T^2 + 17.400T^{-1} + 6.907\times10^{-3}T$

301.55-952 K: $\Delta Hf° = -22.212 - 4.003\times10^{-3}T - 0.472\times10^{-6}T^2 + 133.400T^{-1}$

$\Delta Gf° = -22.212 + 4.003\times10^{-3}T\ln T + 0.472\times10^{-6}T^2 + 66.700T^{-1} - 33.781\times10^{-3}T$

952-2000 K: $\Delta Hf° = -59.283 + 0.745\times10^{-3}T - 0.369\times10^{-6}T^2 + 192.600T^{-1}$

$\Delta Gf° = -59.283 - 0.745\times10^{-3}T\ln T + 0.369\times10^{-6}T^2 + 96.300T^{-1} + 37.788\times10^{-3}T$

Source: Data from JANAF (51) who estimated all except enthalpy of formation at 298 K.

Cu(c,1)

Copper

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.841	7.924	7.924	0
300	5.846	7.961	7.924	.011
400	6.030	9.669	8.156	.605
500	6.190	11.032	8.598	1.217
600	6.330	12.174	9.102	1.843
700	6.450	13.159	9.613	2.482
800	6.570	14.028	10.112	3.133
900	6.690	14.809	10.591	3.796
1000	6.830	15.521	11.049	4.472
1100	7.030	16.181	11.486	5.164
1200	7.270	16.803	11.904	5.879
1300	7.660	17.399	12.303	6.625
1357.6	7.970	17.736	12.524	7.075
1357.6	7.800	20.034	12.524	10.195
1400	7.800	20.274	12.755	10.526
1500	7.800	20.812	13.275	11.306
1600	7.800	21.316	13.762	12.086
1700	7.800	21.788	14.220	12.866
1800	7.800	22.234	14.653	13.646
1900	7.800	22.656	15.063	14.426
2000	7.800	23.056	15.453	15.206
2100	7.800	23.437	15.825	15.986
2200	7.800	23.800	16.179	16.766
2300	7.800	24.146	16.517	17.546
2400	7.800	24.478	16.842	18.326
2500	7.800	24.797	17.155	19.106
2600	7.800	25.103	17.455	19.886
2700	7.800	25.397	17.743	20.666
2800	7.800	25.681	18.022	21.446
2839	7.800	25.788	18.127	21.750

Phase changes: 1357.6 K, melting point of Cu; ΔH° = 3.120 kcal/mol.
2839 K, boiling point of Cu; ΔH° = 71.9 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1357.6 K: $C_p^\circ = 5.320 + 1.620\times10^{-3}T + 0.070\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.320\times10^{-3}T + 0.810\times10^{-6}T^2 - 0.070\times10^{2}T^{-1} - 1.635$

1357.6-2839 K: $C_p^\circ = 7.800$

$H^\circ - H^\circ_{298} = 7.800\times10^{-3}T - 0.394$

Source: Data from King (132).

Cu(g)

Copper (ideal monatomic gas)

[Formation: Cu(c,1) = Cu(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	39.743	39.743	0	80.600	71.113	-52.127
300	4.968	39.774	39.744	.009	80.598	71.054	-51.762
400	4.968	41.203	39.938	.506	80.501	67.887	-37.091
500	4.968	42.312	40.306	1.003	80.386	64.746	-28.300
600	4.968	43.217	40.717	1.500	80.257	61.631	-22.449
700	4.968	43.983	41.132	1.996	80.114	58.537	-18.276
800	4.968	44.646	41.530	2.493	79.960	55.466	-15.152
900	4.968	45.232	41.910	2.990	79.794	52.413	-12.728
1000	4.968	45.755	42.268	3.487	79.615	49.381	-10.792
1100	4.969	46.229	42.607	3.984	79.420	46.367	-9.212
1200	4.970	46.661	42.928	4.480	79.201	43.371	-7.899
1300	4.972	47.059	43.230	4.978	78.953	40.395	-6.791
1357.6	4.975	47.274	43.397	5.264	78.789	38.688	-6.228
1357.6	4.975	47.274	43.397	5.264	75.669	38.688	-6.228
1400	4.977	47.427	43.516	5.475	75.549	37.535	-5.859
1500	4.985	47.771	43.789	5.973	75.267	34.828	-5.074
1600	4.997	48.093	44.048	6.472	74.986	32.143	-4.390
1700	5.016	48.397	44.295	6.973	74.707	29.472	-3.789
1800	5.041	48.684	44.531	7.475	74.429	26.819	-3.256
1900	5.074	48.957	44.756	7.981	74.155	24.183	-2.782
2000	5.116	49.219	44.974	8.491	73.885	21.559	-2.356

Phase change: 1357.6 K, melting point of Cu; $\Delta H° = 3.120$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.952 + 0.024\times10^{-3}T$

$H°- H°_{298} = 4.952\times10^{-3}T + 0.012\times10^{-6}T^2 - 1.478$

Formation equations (kcal/mol):

298.15-1357.6 K: $\Delta Hf° = 80.757 - 0.368\times10^{-3}T - 0.798\times10^{-6}T^2 + 7.000T^{-1}$

$\Delta Gf° = 80.757 + 0.368\times10^{-3}T\ln T + 0.798\times10^{-6}T^2 + 3.500T^{-1} - 34.720\times10^{-3}T$

1357.6-2000 K: $\Delta Hf° = 79.516 - 2.848\times10^{-3}T + 0.012\times10^{-6}T^2$

$\Delta Gf° = 79.516 + 2.848\times10^{-3}T\ln T - 0.012\times10^{-6}T^2 - 50.594\times10^{-3}T$

Source: Data from King (132).

CuO(c)

Copper Oxide

[Formation: $Cu(c,l) + 0.5O_2(g) = CuO(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.109	10.190	10.190	0	-37.200	-30.570	22.408
300	10.141	10.252	10.190	0.019	-37.199	-30.528	22.240
400	11.170	13.327	10.602	1.090	-37.076	-28.322	15.474
500	11.769	15.888	11.410	2.239	-36.905	-26.153	11.431
600	12.224	18.076	12.344	3.439	-36.709	-24.021	8.749
700	12.572	19.988	13.302	4.680	-36.496	-21.922	6.844
800	12.796	21.682	14.246	5.949	-36.277	-19.856	5.424
900	12.920	23.197	15.157	7.236	-36.060	-17.815	4.326
1000	13.020	24.564	16.031	8.533	-35.852	-15.800	3.453
1100	13.197	25.812	16.865	9.842	-35.655	-13.804	2.743
1200	13.539	26.973	17.658	11.178	-35.458	-11.825	2.154
1300	14.133	28.078	18.417	12.559	-35.250	-9.865	1.658
1357.6	14.715	28.700	18.841	13.385	-35.123	-8.746	1.408
1357.6	14.715	28.700	18.841	13.385	-38.243	-8.746	1.408
1400*	15.143	29.159	19.146	14.018	-38.125	-7.826	1.222

*Decomposes above 1400 K.

Phase change: 1357.6 K, melting point of Cu; $\Delta H° = 3.120$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp° = 11.485 + 1.934\times10^{-3}T - 1.736\times10^{5}T^{-2}$

$H°- H°_{298} = 11.485\times10^{-3}T + 0.967\times10^{-6}T^{2} + 1.736\times10^{2}T^{-1} - 4.092$

Formation equations (kcal/mol):

298.15-1357.6 K: $\Delta Hf° = -38.482 + 2.550\times10^{-3}T - 0.095\times10^{-6}T^{2} + 158.000T^{-1}$

$\Delta Gf° = -38.482 - 2.550\times10^{-3}T\ln T + 0.095\times10^{-6}T^{2} + 79.000T^{-1} + 40.148\times10^{-3}T$

1357.6-1400 K: $\Delta Hf° = -39.723 + 0.070\times10^{-3}T + 0.716\times10^{-6}T^{2} + 151.000T^{-1}$

$\Delta Gf° = -39.723 - 0.070\times10^{-3}T\ln T - 0.716\times10^{-6}T^{2} + 75.500T^{-1} + 24.274\times10^{-3}T$

Source: Data from King (132).

CuO(g)

Copper Oxide (ideal gas)

[Formation: $Cu(c,l) + 0.5O_2(g) = CuO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.522	56.072	56.072	0	58.000	50.950	-37.347
300	8.526	56.124	56.072	.016	57.998	50.907	-37.085
400	8.689	58.601	56.409	.877	57.910	48.556	-26.529
500	8.791	60.552	57.048	1.752	57.808	46.228	-20.206
600	8.862	62.161	57.771	2.634	57.687	43.923	-15.999
700	8.921	63.532	58.498	3.524	57.549	41.641	-13.001
800	8.982	64.727	59.203	4.419	57.393	39.378	-10.758
900	9.049	65.789	59.878	5.320	57.224	37.136	-9.018
1000	9.126	66.746	60.517	6.229	57.044	34.914	-7.630
1100	9.211	67.620	61.124	7.146	56.850	32.711	-6.499
1200	9.301	68.425	61.699	8.071	56.635	30.526	-5.559
1300	9.394	69.174	62.246	9.006	56.396	28.357	-4.767
1357.6	9.447	69.582	62.548	9.549	56.241	27.117	-4.365
1357.6	9.447	69.582	62.548	9.549	53.121	27.117	-4.365
1400	9.486	69.873	62.766	9.950	53.007	26.306	-4.106
1500	9.575	70.531	63.262	10.903	52.746	24.407	-3.556
1600	9.658	71.151	63.735	11.865	52.489	22.528	-3.077
1700	9.735	71.739	64.189	12.835	52.238	20.662	-2.656
1800	9.805	72.298	64.625	13.812	51.991	18.812	-2.284
1900	9.867	72.829	65.042	14.795	51.747	16.976	-1.953
2000	9.922	73.337	65.444	15.785	51.508	15.152	-1.656

Phase change: 1357.6 K, melting point of Cu; $\Delta H° = 3.120$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.300 + 0.840\times10^{-3}T + 0.080\times10^{5}T^{-2}$

$H°- H°_{298} = 8.300\times10^{-3}T + 0.420\times10^{-6}T^{2} - 0.080\times10^{2}T^{-1} - 2.485$

Formation equations (kcal/mol):

298.15-1357.6 K: $\Delta Hf° = 58.326 - 0.635\times10^{-3}T - 0.642\times10^{-6}T^{2} - 23.600T^{-1}$

$\Delta Gf° = 58.326 + 0.635\times10^{-3}T\ln T + 0.642\times10^{-6}T^{2} - 11.800T^{-1} - 28.414\times10^{-3}T$

1357.6-2000 K: $\Delta Hf° = 57.085 - 3.115\times10^{-3}T + 0.169\times10^{-6}T^{2} - 30.600T^{-1}$

$\Delta Gf° = 57.085 + 3.115\times10^{-3}T\ln T - 0.169\times10^{-6}T^{2} - 15.300T^{-1} - 44.288\times10^{-3}T$

Source: Data from King (132).

$Cu_2O(c,1)$

Dicopper Oxide

[Formation: $2Cu(c,1) + 0.5O_2(g) = Cu_2O(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.960	22.083	22.083	0	-40.800	-35.354	25.915
300	14.990	22.176	22.083	.028	-40.800	-35.319	25.730
400	16.155	26.653	22.685	1.587	-40.784	-33.492	18.299
500	17.015	30.356	23.860	3.248	-40.713	-31.679	13.847
600	17.640	33.516	25.213	4.982	-40.609	-29.880	10.884
700	18.104	36.272	26.601	6.770	-40.487	-28.102	8.774
800	18.478	38.714	27.964	8.600	-40.359	-26.341	7.196
900	18.830	40.911	29.283	10.465	-40.227	-24.597	5.973
1000	19.226	42.915	30.547	12.368	-40.089	-22.867	4.998
1100	19.738	44.770	31.757	14.314	-39.946	-21.151	4.202
1200	20.444	46.516	32.914	16.322	-39.792	-19.448	3.542
1300	21.434	48.189	34.025	18.413	-39.622	-17.761	2.986
1357.6	22.226	49.133	34.646	19.666	-39.517	-16.800	2.704
1357.6	22.226	49.133	34.646	19.666	-45.757	-16.800	2.704
1400	22.809	49.825	35.096	20.621	-45.647	-15.898	2.482
1500	24.689	51.460	36.133	22.991	-45.272	-13.787	2.009
1516.7	25.063	51.736	36.303	23.407	-45.190	-13.436	1.936
1516.7	23.843	61.858	36.303	38.760	-29.837	-13.436	1.936
1600	23.843	63.132	37.666	40.745	-29.517	-12.542	1.713
1700	23.843	64.577	39.207	43.129	-29.134	-11.495	1.478
1800	23.843	65.940	40.654	45.514	-28.753	-10.467	1.271

Phase changes: 1357.6 K, melting point of Cu; $\Delta H° = 3.120$ kcal/mol.
1516.7 K, melting point of Cu_2O; $\Delta H° = 15.353$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1516.7 K: $Cp° = 14.131 + 5.790\times10^{-3}T - 0.798\times10^{5}T^{-2}$

$H°- H°_{298} = 14.131\times10^{-3}T + 2.895\times10^{-6}T^{2} + 0.798\times10^{2}T^{-1} - 4.738$

1516.7-1800 K: $Cp° = 23.843$

$H°- H°_{298} = 23.843\times10^{-3}T + 2.597$

Formation equations (kcal/mol):

298.15-1357.6 K: $\Delta Hf° = -41.093 - 0.124\times10^{-3}T + 1.023\times10^{-6}T^{2} + 71.200T^{-1}$

$\Delta Gf° = -41.093 + 0.124\times10^{-3}T\ln T - 1.023\times10^{-6}T^{2} + 35.600T^{-1} + 18.448\times10^{-3}T$

1357.6-1516.7 K: $\Delta Hf° = -43.575 - 5.084\times10^{-3}T + 2.643\times10^{-6}T^{2} + 57.200T^{-1}$

$\Delta Gf° = -43.575 + 5.084\times10^{-3}T\ln T - 2.643\times10^{-6}T^{2} + 28.600T^{-1} - 13.300\times10^{-3}T$

1516.7-1800 K: $\Delta Hf° = -36.240 + 4.628\times10^{-3}T - 0.251\times10^{-6}T^{2} - 22.600T^{-1}$

$\Delta Gf° = -36.240 - 4.628\times10^{-3}T\ln T + 0.251\times10^{-6}T^{2} - 11.300T^{-1} + 48.624\times10^{-3}T$

Source: Data from King (132).

Dy(c,l)

Dysprosium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.720	17.900	17.900	0
300	6.720	17.940	17.900	.012
400	6.710	19.870	18.160	.684
500	6.730	21.370	18.658	1.356
600	6.790	22.600	19.215	2.031
700	6.900	23.660	19.783	2.714
800	7.070	24.590	20.324	3.413
900	7.300	25.440	20.850	4.131
1000	7.590	26.220	21.345	4.875
1100	8.000	26.960	21.821	5.653
1200	8.550	27.680	22.280	6.480
1300	9.180	28.390	22.724	7.366
1400	9.870	29.090	23.149	8.317
1500	10.660	29.800	23.571	9.343
1600	11.500	30.510	23.979	10.450
1657	11.990	30.930	24.220	11.119
1657	6.700	31.530	24.220	12.114
1682	6.700	31.630	24.328	12.281
1682	11.930	33.200	24.328	14.924
1700	11.930	33.320	24.415	15.138
1800	11.930	34.010	24.937	16.331
1900	11.930	34.650	25.427	17.524
2000	11.930	35.260	25.901	18.717

Phase changes: 1657 K, α - β transition point of Dy; ΔH° = 0.995 kcal/mol.
1682 K, melting point of Dy; ΔH° = 2.643 kcal/mol.
2835 K, boiling point of Dy; ΔH° = 55.0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1657 K: $Cp^\circ = 3.490 + 4.450\times10^{-3}T + 1.692\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 3.490\times10^{-3}T + 2.225\times10^{-6}T^2 - 1.692\times10^{2}T^{-1} - 0.671$

1657-1682 K: $Cp^\circ = 6.700$

$H^\circ - H^\circ_{298} = 6.700\times10^{-3}T + 1.012$

1682-2000 K: $Cp^\circ = 11.930$

$H^\circ - H^\circ_{298} = 11.930\times10^{-3}T - 5.142$

Source: Data from Hultgren (99).

Dy(g)

Dysprosium (ideal monatomic gas)

[Formation: Dy(c,l) = Dy(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH_f°	ΔG_f°	
298.15	4.968	46.794	46.794	0	69.400	60.785	-44.556
300	4.968	46.825	46.795	.009	69.397	60.732	-44.242
400	4.968	48.254	46.989	.506	69.222	57.868	-31.617
500	4.970	49.363	47.357	1.003	69.047	55.050	-24.062
600	4.976	50.269	47.769	1.500	68.869	52.268	-19.038
700	4.993	51.038	48.184	1.998	68.684	49.519	-15.460
800	5.024	51.706	48.582	2.499	68.486	46.793	-12.783
900	5.070	52.300	48.962	3.004	68.273	44.099	-10.709
1000	5.131	52.838	49.324	3.514	68.039	41.421	-9.052
1100	5.204	53.330	49.666	4.030	67.777	38.770	-7.703
1200	5.285	53.786	49.990	4.555	67.475	36.148	-6.583
1300	5.373	54.213	50.299	5.088	67.122	33.552	-5.641
1400	5.463	54.614	50.593	5.629	66.712	30.978	-4.836
1500	5.555	54.994	50.874	6.180	66.237	28.446	-4.145
1600	5.646	55.356	51.143	6.740	65.690	25.936	-3.543
1657	5.697	55.555	51.292	7.063	65.344	24.541	-3.237
1657	5.697	55.555	51.292	7.063	64.349	24.541	-3.237
1682	5.720	55.640	51.356	7.206	64.325	23.939	-3.110
1682	5.720	55.640	51.356	7.206	61.682	23.939	-3.110
1700	5.736	55.701	51.402	7.309	61.571	23.523	-3.024
1800	5.822	56.031	51.649	7.887	60.956	21.318	-2.588
1900	5.904	56.348	51.888	8.474	60.350	19.124	-2.200
2000	5.982	56.653	52.119	9.068	59.751	16.965	-1.854

Phase changes: 1657 K, α - β transition point of Dy; ΔH° = 0.995 kcal/mol.
1682 K, melting point of Dy; ΔH° = 2.643 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 4.444 + 0.726\times10^{-3}T + 0.274\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.444\times10^{-3}T + 0.363\times10^{-6}T^2 - 0.274\times10^{2}T^{-1} - 1.265$

Formation equations (kcal/mol):

298.15-1657 K: $\Delta H_f^\circ = 68.805 + 0.954\times10^{-3}T - 1.862\times10^{-6}T^2 + 141.800T^{-1}$

$\Delta G_f^\circ = 68.805 - 0.954\times10^{-3}T\ln T + 1.862\times10^{-6}T^2 + 70.900T^{-1} - 22.817\times10^{-3}T$

1657-1682 K: $\Delta H_f^\circ = 67.122 - 2.256\times10^{-3}T + 0.363\times10^{-6}T^2 - 27.400T^{-1}$

$\Delta G_f^\circ = 67.122 + 2.256\times10^{-3}T\ln T - 0.363\times10^{-6}T^2 - 13.700T^{-1} - 41.879\times10^{-3}T$

1682-2000 K: $\Delta H_f^\circ = 73.276 - 7.486\times10^{-3}T + 0.363\times10^{-6}T^2 - 27.400T^{-1}$

$\Delta G_f^\circ = 73.276 + 7.486\times10^{-3}T\ln T - 0.363\times10^{-6}T^2 - 13.700T^{-1} - 84.385\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). All other data from Feber (58).

Dy_2O_3(c)

Didysprosium Trioxide, Dysprosium Sesquioxide

[Formation: $2Dy(c,l) + 1.5O_2(g) = Dy_2O_3(c)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	27.790	35.800	35.800	0	-445.320	-423.404	310.359
300	27.830	35.972	35.802	.051	-445.312	-423.268	308.347
400	29.364	44.198	36.911	2.915	-444.858	-415.987	227.282
500	30.299	50.859	39.055	5.902	-444.311	-408.830	178.697
600	30.877	56.438	41.500	8.963	-443.732	-401.788	146.349
700	31.260	61.229	43.985	12.071	-443.158	-394.833	123.271
800	31.553	65.423	46.408	15.212	-442.612	-387.974	105.988
900	31.822	69.154	48.732	18.380	-442.100	-381.166	92.559
1000	32.114	72.522	50.945	21.577	-441.632	-374.429	81.830
1100	32.454	75.598	53.048	24.805	-441.219	-367.731	73.060
1200	32.850	78.439	55.047	28.070	-440.880	-361.064	65.758
1300	33.293	81.085	56.950	31.376	-440.630	-354.421	59.583
1400	33.756	83.570	58.764	34.729	-440.475	-347.809	54.295
1500	34.198	85.914	60.496	38.127	-440.434	-341.185	49.710
1590	34.528	87.917	61.992	41.220	-440.509	-335.242	46.079
1590	34.400	88.055	61.992	41.440	-440.289	-335.242	46.079
1600	34.400	88.270	62.155	41.784	-440.306	-334.580	45.701
1657	34.400	89.475	63.075	43.745	-440.436	-330.782	43.628
1657	34.400	89.475	63.075	43.745	-442.426	-330.782	43.628
1682	34.400	89.990	63.471	44.605	-442.231	-329.103	42.761
1682	34.400	89.990	63.471	44.605	-447.517	-329.103	42.761
1700	34.400	90.356	63.754	45.224	-447.565	-327.859	42.149
1800	34.400	92.322	65.286	48.664	-447.843	-320.779	38.947
1900	34.400	94.182	66.759	52.104	-448.130	-313.733	36.087
2000	34.400	95.946	68.174	55.544	-448.424	-306.658	33.510

Phase changes: 1590 K, α - β transition point of Dy_2O_3; ΔH° = 0.220 kcal/mol.
1657 K, α - β transition point of Dy; ΔH° = 0.995 kcal/mol.
1682 K, melting point of Dy; ΔH° = 2.643 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1590 K: $Cp° = 29.826 + 2.774\times10^{-3}T - 2.545\times10^{5}T^{-2}$

$H°- H°_{298} = 29.826\times10^{-3}T + 1.387\times10^{-6}T^2 + 2.545\times10^{2}T^{-1} - 9.870$

1590-2000 K: $Cp° = 34.400$

$H°- H°_{298} = 34.400\times10^{-3}T - 13.256$

Formation equations (kcal/mol):

298.15-1590 K: $\Delta Hf° = -450.320 + 12.001\times10^{-3}T - 3.817\times10^{-6}T^2 + 525.100T^{-1}$

$\Delta Gf° = -450.320 - 12.001\times10^{-3}T\ln T + 3.817\times10^{-6}T^2 + 262.550T^{-1} + 154.563\times10^{-3}T$

1590-1657 K: $\Delta Hf° = -453.706 + 16.575\times10^{-3}T - 5.204\times10^{-6}T^2 + 270.600T^{-1}$

$\Delta Gf° = -453.706 - 16.575\times10^{-3}T\ln T + 5.204\times10^{-6}T^2 + 135.300T^{-1} + 188.254\times10^{-3}T$

1657-1682 K: $\Delta Hf° = -457.072 + 10.155\times10^{-3}T - 0.754\times10^{-6}T^2 - 67.800T^{-1}$

$\Delta Gf° = -457.072 - 10.155\times10^{-3}T\ln T + 0.754\times10^{-6}T^2 - 33.900T^{-1} + 150.131\times10^{-3}T$

1682-2000 K: $\Delta Hf° = -444.764 - 0.305\times10^{-3}T - 0.754\times10^{-6}T^2 - 67.800T^{-1}$

$\Delta Gf° = -444.764 + 0.305\times10^{-3}T\ln T + 0.754\times10^{-6}T^2 - 33.900T^{-1} + 65.120\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Huber (97). Low-temperature heat capacities and entropy at 298 K from Westrum (248). High-temperature data based on Pankratz (176).

$e^-(g)$

Electron (ideal gas)

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	4.968	4.988	4.988	0
300	4.968	5.019	4.989	.009
400	4.968	6.448	5.183	.506
500	4.968	7.556	5.550	1.003
600	4.968	8.462	5.962	1.500
700	4.968	9.228	6.377	1.996
800	4.968	9.891	6.775	2.493
900	4.968	10.477	7.155	2.990
1000	4.968	11.000	7.513	3.487
1100	4.968	11.473	7.851	3.984
1200	4.968	11.906	8.173	4.480
1300	4.968	12.303	8.475	4.977
1400	4.968	12.672	8.762	5.474
1500	4.968	13.014	9.033	5.971
1600	4.968	13.335	9.293	6.468
1700	4.968	13.636	9.540	6.964
1800	4.968	13.920	9.775	7.461
1900	4.968	14.189	10.001	7.958
2000	4.968	14.443	10.215	8.455
2100	4.968	14.686	10.423	8.952
2200	4.968	14.917	10.622	9.448
2300	4.968	15.138	10.814	9.945
2400	4.968	15.349	10.998	10.442
2500	4.968	15.552	11.176	10.939
2600	4.968	15.747	11.349	11.436
2700	4.968	15.934	11.515	11.932
2800	4.968	16.115	11.676	12.429
2900	4.968	16.289	11.832	12.926
3000	4.968	16.458	11.984	13.423

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 4.968$

$H^\circ - H^\circ_{298} = 4.968 \times 10^{-3} T - 1.481$

Source: Data from Chase (52).

Er(c,1)

Erbium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.710	17.490	17.490	0
300	6.710	17.530	17.490	.012
400	6.790	19.480	17.760	.688
500	6.870	21.000	18.258	1.371
600	6.970	22.260	18.822	2.063
700	7.110	23.350	19.397	2.767
800	7.270	24.300	19.944	3.485
900	7.460	25.170	20.480	4.221
1000	7.670	25.970	20.993	4.977
1100	7.910	26.710	21.477	5.756
1200	8.180	27.410	21.943	6.560
1300	8.470	28.080	22.394	7.392
1400	8.790	28.720	22.823	8.256
1500	9.140	29.330	23.229	9.152
1600	9.520	29.940	23.637	10.085
1700	9.920	30.530	24.026	11.056
1795	10.330	31.080	24.385	12.017
1795	9.250	33.730	24.385	16.774
1800	9.250	33.750	24.406	16.820
1900	9.250	34.250	24.910	17.746
2000	9.250	34.730	25.395	18.671

Phase changes: 1795 K, melting point of Er; ΔH° = 4.757 kcal/mol.
3136 K, boiling point of Er; ΔH° = 62.5 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1795 K: $Cp^\circ = 5.280 + 2.518\times10^{-3}T + 0.603\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.280\times10^{-3}T + 1.259\times10^{-6}T^2 - 0.603\times10^{2}T^{-1} - 1.484$

1795-2000 K: $Cp^\circ = 9.250$

$H^\circ - H^\circ_{298} = 9.250\times10^{-3}T + 0.170$

Source: Data from Hultgren (99).

Er(g)

Erbium (ideal monatomic gas)

[Formation: Er(c,1) = Er(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	46.347	46.347	0	75.800	67.196	-49.256
300	4.968	46.378	46.348	.009	75.797	67.143	-48.913
400	4.968	47.807	46.542	.506	75.618	64.287	-35.124
500	4.968	48.916	46.910	1.003	75.432	61.474	-26.870
600	4.969	49.822	47.322	1.500	75.237	58.700	-21.381
700	4.973	50.588	47.735	1.997	75.030	55.963	-17.472
800	4.984	51.253	48.134	2.495	74.810	53.248	-14.546
900	5.005	51.841	48.514	2.994	74.573	50.569	-12.280
1000	5.042	52.370	48.874	3.496	74.319	47.919	-10.473
1100	5.100	52.853	49.214	4.003	74.047	45.290	-8.998
1200	5.183	53.300	49.536	4.517	73.757	42.689	-7.775
1300	5.296	53.719	49.842	5.040	73.448	40.117	-6.744
1400	5.441	54.116	50.132	5.577	73.121	37.567	-5.864
1500	5.619	54.498	50.411	6.130	72.778	35.026	-5.103
1600	5.832	54.867	50.678	6.702	72.417	32.534	-4.444
1700	6.077	55.228	50.936	7.297	72.041	30.054	-3.864
1795	6.337	55.565	51.172	7.886	71.669	27.718	-3.375
1795	6.337	55.565	51.172	7.886	66.912	27.718	-3.375
1800	6.351	55.583	51.184	7.918	66.898	27.599	-3.351
1900	6.651	55.934	51.425	8.568	66.622	25.422	-2.924
2000	6.971	56.283	51.659	9.249	66.378	23.272	-2.543

Phase change: 1795 K, melting point of Er; $\Delta H° = 4.757$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.114 + 1.046\times10^{-3}T + 0.482\times10^{5}T^{-2}$

$H°- H°_{298} = 4.114\times10^{-3}T + 0.523\times10^{-6}T^{2} - 0.482\times10^{2}T^{-1} - 1.111$

Formation equations (kcal/mol):

298.15-1795 K: $\Delta Hf° = 76.172 - 1.166\times10^{-3}T - 0.736\times10^{-6}T^{2} + 12.100T^{-1}$

$\Delta Gf° = 76.172 + 1.166\times10^{-3}T\ln T + 0.736\times10^{-6}T^{2} + 6.050T^{-1} - 37.037\times10^{-3}T$

1795-2000 K: $\Delta Hf° = 74.519 - 5.136\times10^{-3}T + 0.523\times10^{-6}T^{2} - 48.200T^{-1}$

$\Delta Gf° = 74.519 + 5.136\times10^{-3}T\ln T - 0.523\times10^{-6}T^{2} - 24.100T^{-1} - 63.593\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). All other data from Feber (59).

$Er_2O_3(c)$

Dierbium Trioxide, Erbium Sesquioxide

[Formation: $2Er(c,1) + 1.5O_2(g) = Er_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	25.930	37.200	37.200	0	-453.590	-432.336	316.906
300	25.979	37.361	37.201	.048	-453.585	-432.204	314.856
400	27.742	45.095	38.243	2.741	-453.310	-425.110	232.266
500	28.773	51.405	40.265	5.570	-452.943	-418.105	182.751
600	29.477	56.716	42.574	8.485	-452.545	-411.175	149.768
700	30.018	61.302	44.929	11.461	-452.143	-404.304	126.228
800	30.466	65.341	47.235	14.485	-451.753	-397.513	108.594
900	30.852	68.952	49.450	17.552	-451.379	-390.749	94.886
1000	31.195	72.220	51.566	20.654	-451.029	-384.024	83.927
1100	31.504	75.208	53.582	23.789	-450.711	-377.344	74.970
1200	31.785	77.962	55.500	26.954	-450.425	-370.685	67.510
1300	32.043	80.516	57.327	30.146	-450.181	-364.039	61.200
1400	32.279	82.899	59.069	33.362	-449.990	-357.421	55.795
1500	32.496	85.134	60.733	36.601	-449.847	-350.839	51.117
1600	32.695	87.238	62.325	39.861	-449.769	-344.216	47.017
1700	32.877	89.225	63.849	43.139	-449.756	-337.614	43.403
1795	33.035	91.017	65.240	46.270	-449.812	-331.345	40.342
1795	33.035	91.017	65.240	46.270	-459.326	-331.345	40.342
1800	33.043	91.109	65.312	46.435	-459.320	-331.009	40.189
1900	33.194	92.900	66.717	49.747	-459.201	-323.888	37.255
2000	33.329	94.606	68.069	53.074	-459.072	-316.746	34.612

Phase change: 1795 K, melting point of Er; $\Delta H° = 4.757$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 28.864 + 2.542\times10^{-3}T - 3.282\times10^{5}T^{-2}$

$H°- H°_{298} = 28.864\times10^{-3}T + 1.271\times10^{-6}T^{2} + 3.282\times10^{2}T^{-1} - 9.820$

Formation equations (kcal/mol):

298.15-1795 K: $\Delta Hf° = -456.914 + 7.459\times10^{-3}T - 2.001\times10^{-6}T^{2} + 381.000T^{-1}$

$\Delta Gf° = -456.914 - 7.459\times10^{-3}T\ln T + 2.001\times10^{-6}T^{2} + 190.500T^{-1} + 122.194\times10^{-3}T$

1795-2000 K: $\Delta Hf° = -460.221 - 0.481\times10^{-3}T + 0.516\times10^{-6}T^{2} + 260.400T^{-1}$

$\Delta Gf° = -460.221 + 0.481\times10^{-3}T\ln T - 0.516\times10^{-6}T^{2} + 130.200T^{-1} + 69.083\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). Entropy at 298 K from Justice (112). Low-temperature heat capacities from Westrum (248). High-temperature data based on Pankratz (178).

Eu(c,l,g)

Europium

T, K	cal/mol•K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.610	18.600	18.600	0
300	6.610	18.641	18.601	.012
400	6.680	20.559	18.867	.677
500	6.920	22.078	19.364	1.357
600	7.240	23.369	19.927	2.065
700	7.520	24.507	20.503	2.803
800	7.880	25.535	21.069	3.573
900	8.440	26.496	21.619	4.389
1000	9.090	27.419	22.154	5.265
1090	9.780	28.231	22.622	6.114
1090	9.110	30.251	22.622	8.316
1100	9.110	30.334	22.691	8.407
1200	9.110	31.127	23.362	9.318
1300	9.110	31.857	23.989	10.229
1400	9.110	32.532	24.575	11.140
1500	9.110	33.161	25.127	12.051
1600	9.110	33.749	25.648	12.962
1700	9.110	34.301	26.140	13.873
1800	9.110	34.820	26.607	14.784
1800	5.019	54.034	26.607	49.369
1900	5.050	54.308	28.060	49.872
2000	5.095	54.568	29.378	50.379

Phase changes: 1090 K, melting point of Eu; ΔH° = 2.202 kcal/mol.
1800 K, boiling point of Eu; ΔH° = 34.585 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1090 K: $Cp^\circ = 4.296 + 4.560\times10^{-3}T + 0.846\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.296\times10^{-3}T + 2.280\times10^{-6}T^2 - 0.846\times10^{2}T^{-1} - 1.200$

1090-1800 K: $Cp^\circ = 9.110$

$H^\circ - H^\circ_{298} = 9.110\times10^{-3}T - 1.614$

1800-2000 K: $Cp^\circ = 4.080 + 0.510\times10^{-3}T$

$H^\circ - H^\circ_{298} = 4.080\times10^{-3}T + 0.255\times10^{-6}T^2 + 41.199$

Source: Gschneidner (89).

Eu(g)

Europium (ideal monatomic gas)

[Formation: Eu(c,l,g) = Eu(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^{\circ}_{298})/T$	$H°-H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	4.968	45.097	45.097	0	41.900	34.000	-24.922
300	4.968	45.127	45.097	.009	41.897	33.951	-24.733
400	4.968	46.557	45.292	.506	41.729	31.330	-17.118
500	4.968	47.665	45.659	1.003	41.546	28.753	-12.568
600	4.968	48.571	46.071	1.500	41.335	26.214	-9.548
700	4.968	49.337	46.486	1.996	41.093	23.712	-7.403
800	4.968	50.000	46.884	2.493	40.820	21.248	-5.805
900	4.968	50.585	47.263	2.990	40.501	18.821	-4.570
1000	4.968	51.109	47.622	3.487	40.122	16.432	-3.591
1090	4.968	51.537	47.927	3.934	39.720	14.317	-2.871
1090	4.968	51.537	47.927	3.934	37.518	14.317	-2.871
1100	4.968	51.582	47.960	3.984	37.477	14.104	-2.802
1200	4.968	52.014	48.281	4.480	37.062	11.998	-2.185
1300	4.969	52.412	48.584	4.977	36.648	9.927	-1.669
1400	4.971	52.780	48.870	5.474	36.234	7.887	-1.231
1500	4.976	53.124	49.143	5.972	35.821	5.877	-.856
1600	4.984	53.445	49.401	6.470	35.408	3.894	-.532
1700	4.997	53.747	49.648	6.969	34.996	1.938	-.249
1800	5.019	54.034	49.885	7.469	34.585	0	0
1800	5.019	54.034	49.885	7.469	0	0	0
1900	5.050	54.308	50.112	7.972	0	0	0
2000	5.095	54.568	50.329	8.479	0	0	0

Phase changes: 1090 K, melting point of Eu; $\Delta H° = 2.202$ kcal/mol.
1800 K, boiling point of Eu; $\Delta H° = 34.585$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.951 + 0.022\times10^{-3}T + 0.009\times10^{5}T^{-2}$

$H°-H^{\circ}_{298} = 4.951\times10^{-3}T + 0.011\times10^{-6}T^{2} - 0.009\times10^{2}T^{-1} - 1.474$

Formation equations (kcal/mol):

298.15-1090 K: $\Delta Hf° = 41.626 + 0.655\times10^{-3}T - 2.269\times10^{-6}T^{2} + 83.700T^{-1}$

$\Delta Gf° = 41.626 - 0.655\times10^{-3}T\ln T + 2.269\times10^{-6}T^{2} + 41.850T^{-1} - 22.992\times10^{-3}T$

1090-1800 K: $\Delta Hf° = 42.040 - 4.159\times10^{-3}T + 0.011\times10^{-6}T^{2} - 0.900T^{-1}$

$\Delta Gf° = 42.040 + 4.159\times10^{-3}T\ln T - 0.011\times10^{-6}T^{2} - 0.450T^{-1} - 54.520\times10^{-3}T$

1800-2000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Sources: Enthalpy of formation at 298 K from Schumm (192). All other data from Feber (58).

EuO(c)

Europium Oxide

[Formation: $Eu(c,l) + 0.5O_2(g) = EuO(c)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.650	19.990	19.990	0	-142.900	-136.009	99.696
300	11.700	20.060	19.990	.022	-142.896	-135.965	99.049
400	12.000	23.480	20.462	1.207	-142.731	-133.682	73.039
500	12.180	26.180	21.346	2.417	-142.567	-131.438	57.451
600	12.300	28.410	22.342	3.641	-142.428	-129.224	47.069
700	12.430	30.320	23.353	4.877	-142.319	-127.035	39.662
800	12.550	31.990	24.333	6.126	-142.239	-124.859	34.110
900	12.710	33.480	25.320	7.344	-142.245	-122.737	29.804
1000	12.890	34.830	26.205	8.625	-142.253	-120.569	26.350
1090	13.043	35.941	26.958	9.791	-142.313	-118.609	23.781
1090	13.043	35.941	26.958	9.791	-144.515	-118.609	23.781
1100	13.060	36.060	27.040	9.922	-144.518	-118.372	23.518
1200	13.230	37.210	27.846	11.237	-144.537	-116.000	21.126
1300	13.400	38.270	28.602	12.569	-144.544	-113.613	19.100
1400	13.580	39.270	29.328	13.919	-144.537	-111.234	17.364
1500	13.750	40.220	30.029	15.286	-144.516	-108.865	15.861
1600	13.920	41.110	30.692	16.669	-144.483	-106.485	14.545
1700	14.090	41.960	31.330	18.071	-144.433	-104.112	13.384

Phase change: 1090 K, melting point of Eu; $\Delta H° = 2.202$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1700 K: $Cp° = 11.675 + 1.270\times10^{-3}T - 0.358\times10^{5}T^{-2}$

$H°- H°_{298} = 11.675\times10^{-3}T + 0.635\times10^{-6}T^{2} + 0.358\times10^{2}T^{-1} - 3.657$

Formation equations (kcal/mol):

298.15-1090 K: $\Delta Hf° = -144.182 + 3.764\times10^{-3}T - 1.897\times10^{-6}T^{2} + 97.800T^{-1}$

$\Delta Gf° = -144.182 - 3.764\times10^{-3}T\ln T + 1.897\times10^{-6}T^{2} + 48.900T^{-1} + 47.741\times10^{-3}T$

1090-1700 K: $\Delta Hf° = -143.768 - 1.050\times10^{-3}T + 0.384\times10^{-6}T^{2} + 13.200T^{-1}$

$\Delta Gf° = -143.768 + 1.050\times10^{-3}T\ln T - 0.384\times10^{-6}T^{2} + 6.600T^{-1} + 16.214\times10^{-3}T$

Sources: Low-temperature heat capacities and entropy at 298 K from Teaney (218). All other data from McMasters (153).

Eu_2O_3(cubic)

Dieuropium Trioxide, Europium Sesquioxide

[Formation: $2Eu(c,l) + 1.5O_2(g) = Eu_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	$C_p°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15*	29.800	33.500	33.500	0	-397.400	-374.381	274.425
300	29.848	33.685	33.502	.055	-397.388	-374.237	272.628
400	31.719	42.557	34.697	3.144	-396.694	-366.616	200.307
500	32.855	49.764	37.012	6.376	-395.919	-359.182	156.996
600	33.693	55.832	39.657	9.705	-395.139	-351.908	128.181
700	34.383	61.079	42.350	13.110	-394.376	-344.761	107.638
800	34.984	65.710	44.986	16.579	-393.644	-337.724	92.261
900	35.527	69.862	47.523	20.105	-392.971	-330.774	80.322
1000	36.027	73.632	49.949	23.683	-392.386	-323.895	70.786
1090	36.446	76.755	52.035	26.944	-391.955	-317.752	63.710
1090	36.446	76.755	52.035	26.944	-396.359	-317.752	63.710
1100	36.493	77.088	52.262	27.309	-396.302	-317.031	62.987
1200	36.930	80.282	54.465	30.980	-395.725	-309.849	56.430
1300	37.341	83.254	56.566	34.694	-395.117	-302.714	50.890
1350	37.538	84.667	57.581	36.566	-394.804	-299.167	48.431

*Entropy and heat capacity at 298 K estimated.

Phase changes: 1090 K, melting point of Eu; $\Delta H°$ = 2.202 kcal/mol.
1350 K, cubic to monclinic transition above 1350 K. Monoclinic form metastable below 1350 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1350 K: $C_p° = 31.861 + 4.436\times10^{-3}T - 3.008\times10^{5}T^{-2}$

$H°- H°_{298} = 31.861\times10^{-3}T + 2.218\times10^{-6}T^2 + 3.008\times10^{2}T^{-1} - 10.705$

Formation equations (kcal/mol):

298.15-1090 K: $\Delta Hf° = -402.178 + 12.424\times10^{-3}T - 3.096\times10^{-6}T^2 + 402.200T^{-1}$

$\Delta Gf° = -402.178 - 12.424\times10^{-3}T\ln T + 3.096\times10^{-6}T^2 + 201.100T^{-1} + 160.834\times10^{-3}T$

1090-1350 K: $\Delta Hf° = -401.350 + 2.796\times10^{-3}T + 1.464\times10^{-6}T^2 + 233.000T^{-1}$

$\Delta Gf° = -401.350 - 2.796\times10^{-3}T\ln T - 1.464\times10^{-6}T^2 + 116.500T^{-1} + 97.779\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Fitzgibbon (62). Entropy and heat capacity at 298 K estimated. High-temperature data based on Pankratz (179).

Eu_2O_3(monoclinic)

Dieuropium Trioxide, Europium Sesquioxide

[Formation: $2Eu(c,l,g) + 1.5O_2(g) = Eu_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	29.100	35.000	35.000	0	-394.700	-372.128	272.774
300	29.143	35.180	35.000	.054	-394.690	-371.987	270.989
400	30.909	43.835	36.167	3.067	-394.072	-364.504	199.153
500	32.032	50.860	38.426	6.217	-393.378	-357.189	156.125
600	32.924	56.781	41.004	9.466	-392.678	-350.016	127.492
700	33.711	61.916	43.633	12.798	-391.988	-342.959	107.075
800	34.445	66.466	46.209	16.206	-391.318	-336.002	91.790
895	35.119	70.368	48.569	19.510	-390.721	-329.467	80.451
895	34.300	70.513	48.569	19.640	-390.591	-329.467	80.451
900	34.346	70.704	48.691	19.812	-390.565	-329.125	79.921
1000	35.134	74.366	51.079	23.287	-390.082	-322.325	70.443
1090	35.684	77.418	53.128	26.476	-389.723	-316.242	63.407
1090	35.684	77.418	53.128	26.476	-394.127	-316.242	63.407
1100	35.745	77.744	53.350	26.833	-394.078	-315.529	62.689
1200	36.237	80.876	55.516	30.432	-393.574	-308.410	56.168
1300	36.644	83.793	57.580	34.077	-393.035	-301.332	50.658
1400*	36.990	86.522	59.551	37.759	-392.471	-294.300	45.942
1500	37.291	89.084	61.435	41.474	-391.883	-287.306	41.860
1600	37.557	91.500	63.240	45.216	-391.278	-280.356	38.294
1700	37.796	93.784	64.970	48.984	-390.655	-273.442	35.153
1800	38.014	95.950	66.631	52.775	-390.018	-266.568	32.365
1800	38.014	95.950	66.631	52.775	-459.188	-266.568	32.365
1900	38.216	98.011	68.229	56.586	-457.724	-255.901	29.435
2000	38.405	99.976	69.767	60.418	-456.255	-245.316	26.807

*Monoclinic form metastable below 1350 K.

Phase changes: 895 K, α - β transition point of Eu_2O_3; ΔH° = 0.130 kcal/mol.
1090 K, melting point of Eu; ΔH° = 2.202 kcal/mol.
1800 K, boiling point of Eu; ΔH° = 34.585 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-895 K:
$$Cp° = 29.989 + 6.024\times10^{-3}T - 2.387\times10^{5}T^{-2}$$
$$H°- H°_{298} = 29.989\times10^{-3}T + 3.012\times10^{-6}T^{2} + 2.387\times10^{2}T^{-1} - 10.010$$

895-2000 K:
$$Cp° = 36.984 + 1.068\times10^{-3}T - 29.157\times10^{5}T^{-2}$$
$$H°- H°_{298} = 36.984\times10^{-3}T + 0.534\times10^{-6}T^{2} + 29.157\times10^{2}T^{-1} - 17.146$$

Formation equations (kcal/mol):

298.15-895 K:
$$\Delta Hf° = -398.782 + 10.552\times10^{-3}T - 2.303\times10^{-6}T^{2} + 340.100T^{-1}$$
$$\Delta Gf° = -398.782 - 10.552\times10^{-3}T\ln T + 2.303\times10^{-6}T^{2} + 170.050T^{-1} + 146.921\times10^{-3}T$$

895-1090 K:
$$\Delta Hf° = -405.919 + 17.547\times10^{-3}T - 4.780\times10^{-6}T^{2} + 3017.100T^{-1}$$
$$\Delta Gf° = -405.919 - 17.547\times10^{-3}T\ln T + 4.780\times10^{-6}T^{2} + 1508.550T^{-1} + 198.549\times10^{-3}T$$

1090-1800 K:
$$\Delta Hf° = -405.091 + 7.919\times10^{-3}T - 0.220\times10^{-6}T^{2} + 2847.900T^{-1}$$
$$\Delta Gf° = -405.091 - 7.919\times10^{-3}T\ln T + 0.220\times10^{-6}T^{2} + 1423.950T^{-1} + 135.494\times10^{-3}T$$

1800-2000 K:
$$\Delta Hf° = -490.716 + 17.979\times10^{-3}T - 0.731\times10^{-6}T^{2} + 2847.900T^{-1}$$
$$\Delta Gf° = -490.716 - 17.979\times10^{-3}T\ln T + 0.731\times10^{-6}T^{2} + 1423.950T^{-1} + 257.551\times10^{-3}T$$

Sources: At 298 K enthalpy of formation from Fitzgibbon (62), entropy from Schumm (192), and heat capacity estimated. High-temperature data based on Pankratz (179).

$F_2(g)$

Fluorine

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	7.481	48.443	48.443	0
300	7.489	48.489	48.443	.014
400	7.883	50.700	48.743	.783
500	8.183	52.493	49.319	1.587
600	8.399	54.005	49.977	2.417
700	8.554	55.312	50.648	3.265
800	8.670	56.462	51.303	4.127
900	8.759	57.489	51.936	4.998
1000	8.829	58.415	52.537	5.878
1100	8.887	59.260	53.111	6.764
1200	8.935	60.035	53.656	7.655
1300	8.976	60.752	54.175	8.550
1400	9.012	61.418	54.668	9.450
1500	9.045	62.041	55.139	10.353
1600	9.074	62.626	55.589	11.259
1700	9.101	63.177	56.020	12.167
1800	9.126	63.698	56.432	13.079
1900	9.150	64.192	56.828	13.992
2000	9.172	64.662	57.208	14.909
2100	9.193	65.110	57.573	15.827
2200	9.214	65.538	57.926	16.747
2300	9.234	65.948	58.265	17.670
2400	9.253	66.341	58.594	18.594
2500	9.272	66.719	58.911	19.520
2600	9.290	67.083	59.218	20.448
2700	9.308	67.434	59.516	21.378
2800	9.326	67.773	59.805	22.310
2900	9.343	68.101	60.086	23.243
3000	9.361	68.418	60.358	24.179

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 8.508 + 0.348\times10^{-3}T - 1.005\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.508\times10^{-3}T + 0.174\times10^{-6}T^2 + 1.005\times10^{2}T^{-1} - 2.889$

Source: Data from JANAF (53).

F(g)

Fluorine (ideal monatomic gas)

[Formation: $0.5F_2(g) = F(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.437	37.917	37.917	0	18.860	14.777	-10.831
300	5.436	37.951	37.918	.010	18.863	14.751	-10.746
400	5.361	39.505	38.130	.550	19.018	13.356	-7.298
500	5.282	40.693	38.529	1.082	19.149	11.925	-5.212
600	5.218	41.650	38.972	1.607	19.259	10.470	-3.814
700	5.169	42.450	39.413	2.126	19.354	8.998	-2.809
800	5.133	43.138	39.837	2.641	19.438	7.512	-2.052
900	5.105	43.741	40.238	3.153	19.514	6.017	-1.461
1000	5.083	44.277	40.614	3.663	19.584	4.515	-.987
1100	5.066	44.761	40.970	4.170	19.648	3.004	-.597
1200	5.052	45.201	41.304	4.676	19.709	1.488	-.271
1300	5.041	45.605	41.620	5.180	19.765	-.033	.005
1400	5.032	45.978	41.918	5.684	19.819	-1.558	.243
1500	5.025	46.325	42.200	6.187	19.871	-3.086	.450
1600	5.018	46.649	42.468	6.689	19.920	-4.618	.631
1700	5.013	46.954	42.724	7.191	19.968	-6.154	.791
1800	5.009	47.240	42.967	7.692	20.013	-7.691	.934
1900	5.005	47.511	43.199	8.192	20.056	-9.233	1.062
2000	5.001	47.767	43.420	8.693	20.099	-10.773	1.177
2100	4.999	48.011	43.633	9.193	20.140	-12.318	1.282
2200	4.996	48.244	43.839	9.692	20.179	-13.866	1.377
2300	4.994	48.466	44.035	10.192	20.217	-15.415	1.465
2400	4.992	48.678	44.223	10.691	20.254	-16.964	1.545
2500	4.990	48.882	44.406	11.190	20.290	-18.516	1.619
2600	4.988	49.078	44.582	11.689	20.325	-20.070	1.687
2700	4.987	49.266	44.752	12.188	20.359	-21.623	1.750
2800	4.986	49.447	44.916	12.687	20.392	-23.177	1.809
2900	4.985	49.622	45.075	13.185	20.424	-24.734	1.864
3000	4.984	49.791	45.230	13.683	20.453	-26.293	1.915

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 5.249 - 0.144\times10^{-3}T + 0.206\times10^{5}T^{-2}$

$H°- H°_{298} = 5.249\times10^{-3}T - 0.072\times10^{-6}T^{2} - 0.206\times10^{2}T^{-1} - 1.489$

Formation equations (kcal/mol):

298.15-3000 K: $\Delta Hf° = 18.815 + 0.995\times10^{-3}T - 0.159\times10^{-6}T^{2} - 70.850T^{-1}$

$\Delta Gf° = 18.815 - 0.995\times10^{-3}T\ln T + 0.159\times10^{-6}T^{2} - 35.425T^{-1} - 7.525\times10^{-3}T$

Source: Data from JANAF (51).

FO(g)

Fluorine Oxide (ideal gas)

[Formation: $0.5F_2(g) + 0.5O_2(g) = FO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.319	51.765	51.765	0	26.000	25.093	-18.394
300	7.326	51.810	51.765	.014	26.000	25.088	-18.277
400	7.694	53.968	52.056	.765	26.012	24.783	-13.541
500	8.007	55.720	52.620	1.550	26.029	24.473	-10.697
600	8.246	57.202	53.262	2.364	26.051	24.160	-8.800
700	8.426	58.488	53.919	3.198	26.072	23.843	-7.444
800	8.562	59.622	54.563	4.047	26.091	23.522	-6.426
900	8.667	60.637	55.183	4.909	26.111	23.201	-5.634
1000	8.750	61.554	55.774	5.780	26.128	22.877	-5.000
1100	8.818	62.392	56.339	6.658	26.144	22.550	-4.480
1200	8.875	63.161	56.875	7.543	26.159	22.224	-4.047
1300	8.923	63.874	57.387	8.433	26.173	21.895	-3.681
1400	8.965	64.537	57.874	9.328	26.186	21.564	-3.366
1500	9.002	65.156	58.339	10.226	26.198	21.235	-3.094
1600	9.035	65.738	58.783	11.128	26.209	20.904	-2.855
1700	9.066	66.287	59.209	12.033	26.219	20.572	-2.645
1800	9.093	66.806	59.617	12.941	26.227	20.240	-2.457
1900	9.119	67.298	60.007	13.852	26.234	19.908	-2.290
2000	9.144	67.767	60.384	14.765	26.239	19.573	-2.139

*All data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.068 + 0.674\times10^{-3}T - 0.844\times10^{5}T^{-2}$

$H°- H°_{298} = 8.068\times10^{-3}T + 0.337\times10^{-6}T^{2} + 0.844\times10^{2}T^{-1} - 2.719$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 25.902 + 0.199\times10^{-3}T - 0.001\times10^{-6}T^{2} + 11.550T^{-1}$

$\Delta Gf° = 25.902 - 0.199\times10^{-3}T\ln T + 0.001\times10^{-6}T^{2} + 5.775T^{-1} - 1.644\times10^{-3}T$

Source: Data estimated by JANAF (51).

$FO_2(g)$

Fluorine Dioxide (ideal gas)

[Formation: $0.5F_2(g) + O_2(g) = FO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	10.611	61.903	61.903	0	3.000	6.376	-4.674
300	10.626	61.968	61.903	.020	3.000	6.398	-4.661
400	11.319	65.125	62.327	1.119	3.004	7.531	-4.114
500	11.843	67.710	63.154	2.278	3.031	8.659	-3.785
600	12.247	69.907	64.102	3.483	3.066	9.781	-3.563
700	12.559	71.819	65.070	4.724	3.104	10.898	-3.402
800	12.800	73.512	66.021	5.993	3.144	12.008	-3.280
900	12.986	75.031	66.940	7.282	3.184	13.113	-3.184
1000	13.132	76.407	67.818	8.589	3.224	14.215	-3.107
1100	13.248	77.665	68.658	9.908	3.261	15.312	-3.042
1200	13.341	78.821	69.456	11.238	3.297	16.407	-2.988
1300	13.416	79.892	70.218	12.576	3.332	17.498	-2.942
1400	13.478	80.889	70.946	13.920	3.362	18.584	-2.901
1500	13.529	81.821	71.640	15.271	3.391	19.670	-2.866
1600	13.572	82.695	72.304	16.626	3.417	20.756	-2.835
1700	13.608	83.519	72.940	17.985	3.440	21.839	-2.808
1800	13.639	84.298	73.550	19.347	3.457	22.921	-2.783
1900	13.665	85.036	74.134	20.713	3.473	24.003	-2.761
2000	13.688	85.738	74.698	22.080	3.483	25.081	-2.741

*Enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.894 + 1.202\times10^{-3}T - 1.459\times10^{5}T^{-2}$

$H°- H°_{298} = 11.894\times10^{-3}T + 0.601\times10^{-6}T^{2} + 1.459\times10^{2}T^{-1} - 4.089$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 2.708 + 0.410\times10^{-3}T + 0.011\times10^{-6}T^{2} + 50.450T^{-1}$

$\Delta Gf° = 2.708 - 0.410\times10^{-3}T\ln T - 0.011\times10^{-6}T^{2} + 25.225T^{-1} + 14.360\times10^{-3}T$

Source: Data from JANAF (51) who estimated enthalpy of formation at 298 K.

$F_2O(g)$

Difluorine Oxide (ideal gas)

[Formation: $F_2(g) + 0.5O_2(g) = F_2O(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.349	59.118	59.118	0	5.860	9.983	-7.317
300	10.371	59.182	59.119	.019	5.859	10.008	-7.291
400	11.373	62.311	59.539	1.109	5.825	11.398	-6.228
500	12.061	64.928	60.362	2.283	5.829	12.792	-5.591
600	12.524	67.170	61.313	3.514	5.853	14.183	-5.166
700	12.841	69.126	62.293	4.783	5.885	15.568	-4.861
800	13.065	70.856	63.257	6.079	5.920	16.948	-4.630
900	13.227	72.405	64.189	7.394	5.957	18.326	-4.450
1000	13.348	73.805	65.082	8.723	5.992	19.697	-4.305
1100	13.439	75.082	65.935	10.062	6.026	21.066	-4.185
1200	13.511	76.254	66.746	11.410	6.059	22.433	-4.085
1300	13.567	77.338	67.520	12.764	6.090	23.796	-4.000
1400	13.613	78.345	68.257	14.123	6.116	25.156	-3.927
1500	13.650	79.286	68.962	15.486	6.142	26.514	-3.863
1600	13.681	80.168	69.635	16.853	6.164	27.872	-3.807
1700	13.706	80.998	70.279	18.222	6.184	29.229	-3.758
1800	13.728	81.782	70.896	19.594	6.200	30.585	-3.713
1900	13.746	82.524	71.488	20.968	6.214	31.941	-3.674
2000	13.762	83.230	72.059	22.343	6.222	33.293	-3.638

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.684 + 0.750\times10^{-3}T - 2.274\times10^{5}T^{-2}$

$H°- H°_{298} = 12.684\times10^{-3}T + 0.375\times10^{-6}T^{2} + 2.274\times10^{2}T^{-1} - 4.578$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 5.347 + 0.561\times10^{-3}T - 0.050\times10^{-6}T^{2} + 104.300T^{-1}$

$\Delta Gf° = 5.347 - 0.561\times10^{-3}T\ln T + 0.050\times10^{-6}T^{2} + 52.150T^{-1} + 18.141\times10^{-3}T$

Source: Data from JANAF (51).

Fe(c,l)

Iron

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.970	6.520	6.520	0
300	5.980	6.557	6.520	.011
400	6.540	8.354	6.762	.637
500	7.100	9.873	7.235	1.319
600	7.660	11.216	7.789	2.056
700	8.270	12.441	8.368	2.851
800	9.070	13.594	8.949	3.716
900	10.280	14.726	9.528	4.678
1000	12.950	15.920	10.106	5.814
1043	20.000	16.540	10.358	6.448
1100	11.140	17.193	10.697	7.146
1185	9.900	17.967	11.191	8.030
1185	8.080	18.149	11.191	8.245
1200	8.110	18.250	11.278	8.367
1300	8.310	18.907	11.840	9.187
1400	8.510	19.530	12.367	10.028
1500	8.710	20.124	12.865	10.889
1600	8.910	20.693	13.337	11.770
1667	9.050	21.061	13.639	12.372
1667	9.830	21.181	13.639	12.572
1700	9.890	21.374	13.788	12.897
1800	10.130	21.946	14.225	13.897
1811	10.170	22.008	14.271	14.012
1811	11.000	23.830	14.271	17.312
1900	11.000	24.358	14.731	18.291
2000*	11.000	24.922	15.227	19.391
2100	11.000	25.458	15.700	20.491
2200	11.000	25.970	16.156	21.591
2300	11.000	26.459	16.593	22.691
2400	11.000	26.927	17.014	23.791
2500	11.000	27.376	17.420	24.891
2600	11.000	27.808	17.811	25.991
2700	11.000	28.223	18.189	27.091
2800	11.000	28.623	18.555	28.191
2900	11.000	29.009	18.909	29.291
3000	11.000	29.382	19.252	30.391

*Data extrapolated above 1900 K.

Phase changes: 1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1811 K, melting point of Fe; ΔH° = 3.300 kcal/mol.
3135 K, boiling point of Fe; ΔH° = 83.6 kcal/mol.

Fe(c,1) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1043 K: $Cp^\circ = -0.221 + 12.142\times10^{-3}T + 2.285\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = -0.221\times10^{-3}T + 6.071\times10^{-6}T^2 - 2.285\times10^{2}T^{-1} + 0.293$

1043-1185 K: $Cp^\circ = 43.760 - 29.280\times10^{-3}T$

$H^\circ - H^\circ_{298} = 43.760\times10^{-3}T - 14.640\times10^{-6}T^2 - 23.268$

1185-1667 K: $Cp^\circ = 5.505 + 2.102\times10^{-3}T + 1.190\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.505\times10^{-3}T + 1.051\times10^{-6}T^2 - 1.190\times10^{2}T^{-1} + 0.346$

1667-1811 K: $Cp^\circ = -42.992 + 21.364\times10^{-3}T + 478.182\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = -42.992\times10^{-3}T + 10.682\times10^{-6}T^2 - 478.182\times10^{2}T^{-1} + 83.241$

1811-3000 K: $Cp^\circ = 11.000$

$H^\circ - H^\circ_{298} = 11.000\times10^{-3}T - 2.609$

Source: Data from Hultgren (99) who extrapolated above 1900 K by assuming constant heat capacity. Data corrected to IPTS-68.

Fe(g)

Iron (ideal monatomic gas)

[Formation: Fe(c,l) = Fe(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	6.136	43.112	43.112	0	99.300	88.390	-64.791
300	6.138	43.150	43.113	.011	99.300	88.322	-64.342
400	6.102	44.915	43.353	.625	99.288	84.664	-46.257
500	5.949	46.261	43.805	1.228	99.209	81.015	-35.411
600	5.784	47.331	44.308	1.814	99.058	77.389	-28.189
700	5.643	48.212	44.803	2.386	98.835	73.795	-23.040
800	5.529	48.957	45.277	2.944	98.528	70.238	-19.188
900	5.441	49.603	45.723	3.492	98.114	66.725	-16.203
1000	5.375	50.173	46.140	4.033	97.519	63.266	-13.827
1043	5.355	50.399	46.311	4.264	97.116	61.801	-12.950
1100	5.329	50.683	46.530	4.568	96.722	59.883	-11.898
1185	5.306	51.078	46.842	5.019	96.289	57.053	-10.522
1185	5.306	51.078	46.842	5.019	96.074	57.053	-10.522
1200	5.302	51.145	46.896	5.099	96.032	56.558	-10.300
1300	5.291	51.569	47.239	5.629	95.742	53.281	-8.957
1400	5.295	51.961	47.562	6.158	95.430	50.027	-7.809
1500	5.313	52.327	47.868	6.688	95.099	46.795	-6.818
1600	5.343	52.671	48.158	7.221	94.751	43.586	-5.954
1667	5.370	52.891	48.344	7.580	94.508	41.448	-5.434
1667	5.370	52.891	48.344	7.580	94.308	41.448	-5.434
1700	5.383	52.996	48.433	7.757	94.160	40.403	-5.194
1800	5.432	53.305	48.695	8.298	93.701	37.255	-4.523
1811	5.438	53.338	48.723	8.358	93.646	36.907	-4.454
1811	5.438	53.338	48.723	8.358	90.346	36.907	-4.454
1900	5.487	53.600	48.945	8.844	89.853	34.293	-3.945
2000	5.548	53.883	49.185	9.396	89.305	31.383	-3.429
2100	5.613	54.155	49.415	9.954	88.763	28.499	-2.966
2200	5.681	54.418	49.637	10.518	88.227	25.641	-2.547
2300	5.751	54.672	49.850	11.090	87.699	22.809	-2.167
2400	5.823	54.919	50.057	11.669	87.178	19.997	-1.821
2500	5.896	55.158	50.256	12.255	86.664	17.209	-1.504
2600	5.969	55.390	50.448	12.848	86.157	14.444	-1.214
2700	6.042	55.617	50.636	13.448	85.657	11.693	-.946
2800	6.116	55.838	50.818	14.056	85.165	8.963	-.700
2900	6.190	56.054	50.995	14.671	84.680	6.250	-.471
3000	6.264	56.265	51.167	15.294	84.203	3.554	-.259

Phase changes: 1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1811 K, melting point of Fe; ΔH° = 3.300 kcal/mol.

Fe(g) - Continued

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 5.847 - 0.334\times10^{-3}T + 0.345\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.847\times10^{-3}T - 0.167\times10^{-6}T^2 - 0.345\times10^{2}T^{-1} - 1.613$

2000-3000 K: $Cp^\circ = 3.259 + 0.958\times10^{-3}T + 14.886\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 3.259\times10^{-3}T + 0.479\times10^{-6}T^2 - 14.886\times10^{2}T^{-1} + 1.706$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = 97.395 + 6.068\times10^{-3}T - 6.238\times10^{-6}T^2 + 194.000T^{-1}$

$\Delta Gf^\circ = 97.395 - 6.068\times10^{-3}T\ln T + 6.238\times10^{-6}T^2 + 97.000T^{-1} + 1.420\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = 120.955 - 37.913\times10^{-3}T + 14.473\times10^{-6}T^2 - 34.500T^{-1}$

$\Delta Gf^\circ = 120.955 + 37.913\times10^{-3}T\ln T - 14.473\times10^{-6}T^2 - 17.250T^{-1} - 305.124\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = 97.342 + 0.342\times10^{-3}T - 1.218\times10^{-6}T^2 + 84.500T^{-1}$

$\Delta Gf^\circ = 97.342 - 0.342\times10^{-3}T\ln T + 1.218\times10^{-6}T^2 + 42.250T^{-1} - 33.083\times10^{-3}T$

1667-1811 K: $\Delta Hf^\circ = 14.447 + 48.839\times10^{-3}T - 10.849\times10^{-6}T^2 + 47783.700T^{-1}$

$\Delta Gf^\circ = 14.447 - 48.839\times10^{-3}T\ln T + 10.849\times10^{-6}T^2 + 23891.850T^{-1} + 351.795\times10^{-3}T$

1811-2000 K: $\Delta Hf^\circ = 100.297 - 5.153\times10^{-3}T - 0.167\times10^{-6}T^2 - 34.500T^{-1}$

$\Delta Gf^\circ = 100.297 + 5.153\times10^{-3}T\ln T + 0.167\times10^{-6}T^2 - 17.250T^{-1} - 74.003\times10^{-3}T$

2000-3000 K: $\Delta Hf^\circ = 103.616 - 7.741\times10^{-3}T + 0.479\times10^{-6}T^2 - 1488.600T^{-1}$

$\Delta Gf^\circ = 103.616 + 7.741\times10^{-3}T\ln T - 0.479\times10^{-6}T^2 - 744.300T^{-1} - 93.860\times10^{-3}T$

Source: Data from JANAF (55).

$Fe_{.9470}O(c,1)$

Iron Oxide, Wustite

[Formation: $0.947Fe(c) + 0.5O_2(g) = Fe_{.9470}O(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.470	13.740	13.740	0	-63.640	-58.590	42.947
300	11.480	13.811	13.741	.021	-63.636	-58.559	42.660
400	12.110	17.210	14.202	1.203	-63.402	-56.903	31.090
500	12.510	19.960	15.088	2.436	-63.180	-55.305	24.173
600	12.760	22.260	16.092	3.701	-62.991	-53.745	19.576
700	12.930	24.240	17.117	4.986	-62.847	-52.215	16.302
800	13.060	25.980	18.124	6.285	-62.767	-50.708	13.853
900*	13.200	27.520	19.078	7.598	-62.772	-49.195	11.946
1000	13.380	28.920	19.993	8.927	-62.932	-47.681	10.420
1043	13.479	29.485	20.373	9.504	-63.134	-47.021	9.853
1100	13.610	30.210	20.868	10.276	-63.264	-46.140	9.167
1185	13.840	31.226	21.570	11.442	-63.295	-44.809	8.264
1185	13.840	31.226	21.570	11.442	-63.499	-44.809	8.264
1200	13.880	31.400	21.692	11.650	-63.470	-44.574	8.118
1300	14.180	32.530	22.489	13.053	-63.272	-43.016	7.232
1400	14.490	33.590	23.242	14.487	-63.066	-41.462	6.472
1500	14.750	34.600	23.967	15.950	-62.853	-39.927	5.817
1600	14.910	35.560	24.664	17.434	-62.642	-38.409	5.246
1652	14.930	36.030	25.005	18.210	-62.537	-37.608	4.975
1652	16.190	40.560	25.005	25.701	-55.046	-37.608	4.975
1667	16.190	40.706	25.143	25.944	-54.998	-37.446	4.909
1667	16.190	40.706	25.143	25.944	-55.187	-37.446	4.909
1700	16.190	41.030	25.455	26.478	-55.106	-37.107	4.770
1800	16.190	41.960	26.351	28.096	-54.879	-36.063	4.379

*Unstable below 833 K.

Phase changes: 1043 K, Curie temperature of Fe; $\Delta H° = 0$ kcal/mol.
1185 K, $\alpha - \gamma$ transition point of Fe; $\Delta H° = 0.215$ kcal/mol.
1652 K, melting point of $Fe_{.9470}O$; $\Delta H° = 7.491$ kcal/mol.
1667 K, $\gamma - \delta$ transition point of Fe; $\Delta H° = 0.200$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1652 K: $Cp° = 11.823 + 1.836\times10^{-3}T - 0.800\times10^{5}T^{-2}$

$H°- H°_{298} = 11.823\times10^{-3}T + 0.918\times10^{-6}T^2 + 0.800\times10^{2}T^{-1} - 3.875$

1652-1800 K: $Cp° = 16.190$

$H°- H°_{298} = 16.190\times10^{-3}T - 1.045$

$Fe_{.947}O$(c,1) - Continued

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -66.616 + 8.417\times10^{-3}T - 5.083\times10^{-6}T^2 + 273.789T^{-1}$

$\Delta Gf^\circ = -66.616 - 8.417\times10^{-3}T\ln T + 5.083\times10^{-6}T^2 + 136.895T^{-1} + 71.822\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -44.304 - 33.233\times10^{-3}T + 14.531\times10^{-6}T^2 + 57.400T^{-1}$

$\Delta Gf^\circ = -44.304 + 33.233\times10^{-3}T\ln T - 14.531\times10^{-6}T^2 + 28.700T^{-1} - 218.476\times10^{-3}T$

1185-1652 K: $\Delta Hf^\circ = -66.666 + 2.995\times10^{-3}T - 0.329\times10^{-6}T^2 + 170.093T^{-1}$

$\Delta Gf^\circ = -66.666 - 2.995\times10^{-3}T\ln T + 0.329\times10^{-6}T^2 + 85.047T^{-1} + 39.147\times10^{-3}T$

1652-1667 K: $\Delta Hf^\circ = -63.836 + 7.362\times10^{-3}T - 1.247\times10^{-6}T^2 + 90.093T^{-1}$

$\Delta Gf^\circ = -63.836 - 7.362\times10^{-3}T\ln T + 1.247\times10^{-6}T^2 + 45.047T^{-1} + 68.290\times10^{-3}T$

1667-1800 K: $\Delta Hf^\circ = -142.337 + 53.288\times10^{-3}T - 10.367\times10^{-6}T^2 + 45261.234T^{-1}$

$\Delta Gf^\circ = -142.337 - 53.288\times10^{-3}T\ln T + 10.367\times10^{-6}T^2 + 22630.617T^{-1} + 432.770\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (237). High-temperature data based on Coughlin (43) corrected to IPTS-68.

FeO(c)

Iron Oxide

[Formation: Fe(c) + $0.5O_2$(g) = FeO(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.930	14.520	14.520	0	-65.000	-60.080	44.039
300	11.950	14.594	14.521	.022	-64.995	-60.049	43.745
400	12.390	18.094	14.994	1.240	-64.758	-58.436	31.928
500	12.760	20.898	15.904	2.497	-64.549	-56.881	24.862
600	13.120	23.257	16.937	3.792	-64.368	-55.364	20.166
700	13.420	25.303	17.990	5.119	-64.226	-53.875	16.820
800	13.700	27.113	19.019	6.475	-64.133	-52.405	14.316
900	13.930	28.740	20.010	7.857	-64.120	-50.940	12.370
1000	14.190	30.222	20.959	9.263	-64.264	-49.471	10.812
1043	14.279	30.821	21.353	9.875	-64.466	-48.831	10.232
1100	14.396	31.584	21.864	10.692	-64.587	-47.972	9.531
1185	14.569	32.662	22.600	11.923	-64.599	-46.686	8.610
1185	14.569	32.662	22.600	11.923	-64.814	-46.686	8.610
1200	14.600	32.845	22.727	12.142	-64.782	-46.459	8.461
1300	14.813	34.022	23.550	13.613	-64.559	-44.940	7.555
1400	15.000	35.127	24.338	15.104	-64.340	-43.439	6.781
1500	15.151	36.167	25.093	16.611	-64.130	-41.954	6.113
1600	15.300	37.150	25.816	18.134	-63.926	-40.482	5.530

*Stoichiometric FeO does not exist as a stable phase; however $Fe_{.947}O$ exists above 833 K in the wustite region of the Fe-O system.

Phase changes: 1043 K, Curie temperature of Fe; $\Delta H° = 0$ kcal/mol.
1185 K, $\alpha - \gamma$ transition point of Fe; $\Delta H° = 0.215$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp° = 11.764 + 2.430\times10^{-3}T - 0.496\times10^{5}T^{-2}$

$H°- H°_{298} = 11.764\times10^{-3}T + 1.215\times10^{-6}T^{2} + 0.496\times10^{2}T^{-1} - 3.782$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf° = -67.898 + 8.370\times10^{-3}T - 5.108\times10^{-6}T^{2} + 255.500T^{-1}$

$\Delta Gf° = -67.898 - 8.370\times10^{-3}T\ln T + 5.108\times10^{-6}T^{2} + 127.750T^{-1} + 70.953\times10^{-3}T$

1043-1185 K: $\Delta Hf° = -44.338 - 35.611\times10^{-3}T + 15.604\times10^{-6}T^{2} + 27.000T^{-1}$

$\Delta Gf° = -44.338 + 35.611\times10^{-3}T\ln T - 15.604\times10^{-6}T^{2} + 13.500T^{-1} - 235.592\times10^{-3}T$

1185-1600 K: $\Delta Hf° = -67.952 + 2.644\times10^{-3}T - 0.087\times10^{-6}T^{2} + 146.000T^{-1}$

$\Delta Gf° = -67.952 - 2.644\times10^{-3}T\ln T + 0.087\times10^{-6}T^{2} + 73.000T^{-1} + 36.449\times10^{-3}T$

Source: Data from JANAF (51).

Fe_2O_3(c)

Diiron Trioxide, Hematite

[Formation: $2Fe(c) + 1.5O_2(g) = Fe_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.800	20.890	20.890	0	-197.000	-177.424	130.054
300	24.896	21.040	20.890	.046	-196.995	-177.301	129.162
400	28.910	28.840	21.930	2.764	-196.595	-170.793	93.316
500	31.450	35.580	24.000	5.790	-196.029	-164.405	71.861
600	33.370	41.490	26.433	9.034	-195.392	-158.139	57.601
700	35.240	46.770	28.967	12.462	-194.720	-151.981	47.450
800	37.440	51.620	31.504	16.093	-194.016	-145.930	39.866
900	41.460	56.220	33.993	20.004	-193.251	-139.961	33.987
960	47.360	59.060	35.468	22.648	-192.627	-136.426	31.058
960	34.060	59.060	35.468	22.648	-192.627	-136.426	31.058
1000	34.050	60.450	36.440	24.010	-192.757	-134.082	29.303
1043	34.050	61.884	37.460	25.474	-193.100	-131.553	27.565
1100	34.050	63.700	38.776	27.416	-193.273	-128.185	25.468
1185	34.042	66.232	40.654	30.309	-193.228	-123.154	22.713
1185	34.042	66.232	40.654	30.309	-193.658	-123.154	22.713
1200	34.040	66.660	40.977	30.820	-193.584	-122.265	22.267
1300	34.040	69.380	43.054	34.224	-193.104	-116.334	19.557
1400	34.030	71.900	45.023	37.628	-192.678	-110.442	17.241
1500	34.030	74.250	46.896	41.031	-192.302	-104.585	15.238
1600	34.020	76.450	48.679	44.433	-191.977	-98.754	13.489
1667	34.020	77.843	49.821	46.712	-191.787	-94.851	12.435
1667	34.020	77.843	49.821	46.712	-192.187	-94.851	12.435
1700*	34.020	78.510	50.372	47.835	-192.152	-92.925	11.946
1800	34.010	80.450	51.986	51.236	-192.083	-87.080	10.573

*Decomposes near 1700 K.

Phase changes: 960 K, Curie temperature of Fe_2O_3; $\Delta H° = 0$ kcal/mol.
1043 K, Curie temperature of Fe; $\Delta H° = 0$ kcal/mol.
1185 K, $\alpha - \gamma$ transition point of Fe; $\Delta H° = 0.215$ kcal/mol.
1667 K, $\gamma - \delta$ transition point of Fe; $\Delta H° = 0.200$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-960 K: $Cp° = 23.470 + 19.268\times10^{-3}T - 3.927\times10^{5}T^{-2}$

$H°- H°_{298} = 23.470\times10^{-3}T + 9.634\times10^{-6}T^{2} + 3.927\times10^{2}T^{-1} - 9.171$

960-1800 K: $Cp° = 34.040$

$H°- H°_{298} = 34.040\times10^{-3}T - 10.030$

Fe_2O_3(c) - Continued

Formation equations (kcal/mol):

298.15-960 K: $\Delta Hf° = -203.228 + 13.067\times10^{-3}T - 3.263\times10^{-6}T^2 + 781.900T^{-1}$

$\Delta Gf° = -203.228 - 13.067\times10^{-3}T\ln T + 3.263\times10^{-6}T^2 + 390.950T^{-1} + 155.628\times10^{-3}T$

960-1043 K: $\Delta Hf° = -204.088 + 23.637\times10^{-3}T - 12.897\times10^{-6}T^2 + 389.200T^{-1}$

$\Delta Gf° = -204.088 - 23.637\times10^{-3}T\ln T + 12.897\times10^{-6}T^2 + 194.600T^{-1} + 220.071\times10^{-3}T$

1043-1185 K: $\Delta Hf° = -156.966 - 64.325\times10^{-3}T + 28.525\times10^{-6}T^2 - 67.800T^{-1}$

$\Delta Gf° = -156.966 + 64.325\times10^{-3}T\ln T - 28.525\times10^{-6}T^2 - 33.900T^{-1} - 393.018\times10^{-3}T$

1185-1667 K: $\Delta Hf° = -204.194 + 12.185\times10^{-3}T - 2.857\times10^{-6}T^2 + 170.200T^{-1}$

$\Delta Gf° = -204.194 - 12.185\times10^{-3}T\ln T + 2.857\times10^{-6}T^2 + 85.100T^{-1} + 151.063\times10^{-3}T$

1667-1800 K: $\Delta Hf° = -369.984 + 109.179\times10^{-3}T - 22.118\times10^{-6}T^2 + 95568.600T^{-1}$

$\Delta Gf° = -369.984 - 109.179\times10^{-3}T\ln T + 22.118\times10^{-6}T^2 + 47784.301T^{-1} + 920.820\times10^{-3}T$

Sources: Enthalpy of formation from Wagman (237). Low-temperature heat capacities and entropy at 298 K from Gronvold (87). High-temperature data based on Coughlin (43).

$Fe_3O_4(c)$

Triiron Tetroxide, Magnetite

[Formation: $3Fe(c) + 2O_2(g) = Fe_3O_4(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	36.040	34.930	34.930	0	-267.300	-242.661	177.873
300	36.209	35.147	34.930	.067	-267.292	-242.505	176.663
400	41.977	46.412	36.427	3.994	-266.663	-234.331	128.031
500	46.078	56.240	39.428	8.406	-265.759	-226.348	98.936
600	49.744	64.959	42.969	13.194	-264.692	-218.562	79.610
700	54.806	72.975	46.688	18.401	-263.426	-210.968	65.866
800	63.717	80.817	50.463	24.283	-261.735	-203.587	55.617
850	81.000	85.027	52.363	27.764	-260.454	-199.982	51.418
850	54.946	85.027	52.363	27.764	-260.454	-199.982	51.418
900	52.756	88.103	54.265	30.454	-260.078	-196.436	47.701
1000	49.693	93.490	57.927	35.563	-260.031	-189.381	41.389
1043	48.913	95.566	59.436	37.683	-260.532	-186.335	39.044
1100	47.878	98.133	61.375	40.434	-260.834	-182.265	36.212
1185	47.057	101.661	64.139	44.463	-260.897	-176.190	32.494
1185	47.057	101.661	64.139	44.463	-261.542	-176.190	32.494
1200	46.912	102.252	64.612	45.168	-261.459	-175.114	31.892
1300	46.545	105.989	67.654	49.836	-260.963	-167.938	28.233
1400	46.612	109.439	70.517	54.491	-260.559	-160.799	25.102
1500	47.001	112.666	73.220	59.169	-260.204	-153.686	22.392
1600	47.634	115.719	75.782	63.899	-259.871	-146.594	20.024
1667	48.185	117.683	77.426	67.108	-259.648	-141.855	18.597
1667	48.185	117.683	77.426	67.108	-260.248	-141.855	18.597
1700	48.456	118.630	78.216	68.703	-260.212	-139.512	17.935
1800	49.425	121.427	80.540	73.596	-260.095	-132.412	16.077

Phase changes: 850 K, Curie temperature of Fe_3O_4; $\Delta H° = 0$ kcal/mol.
1043 K, Curie temperature of Fe; $\Delta H° = 0$ kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H° = 0.215$ kcal/mol.
1667 K, γ - δ transition point of Fe; $\Delta H° = 0.200$ kcal/mol.
1870 K, melting point of Fe_3O_4; $\Delta H° = 33.0 \pm 2.$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-850 K:

$$Cp° = 19.063 + 53.872\times10^{-3}T + 0.813\times10^{5}T^{-2}$$

$$H°- H°_{298} = 19.063\times10^{-3}T + 26.936\times10^{-6}T^{2} - 0.813\times10^{2}T^{-1} - 7.805$$

850-1800 K:

$$Cp° = 11.915 + 17.332\times10^{-3}T + 204.451\times10^{5}T^{-2}$$

$$H°- H°_{298} = 11.915\times10^{-3}T + 8.666\times10^{-6}T^{2} - 204.451\times10^{2}T^{-1} + 35.428$$

Fe_3O_4(c) - Continued

Formation equations (kcal/mol):

298.15-850 K: $\Delta Hf^\circ = -271.279 + 5.266\times10^{-3}T + 7.717\times10^{-6}T^2 + 513.800T^{-1}$

$\Delta Gf^\circ = -271.279 - 5.266\times10^{-3}T\ln T - 7.717\times10^{-6}T^2 + 256.900T^{-1} + 125.401\times10^{-3}T$

850-1043 K: $\Delta Hf^\circ = -228.046 - 1.882\times10^{-3}T - 10.553\times10^{-6}T^2 - 19850.000T^{-1}$

$\Delta Gf^\circ = -228.046 + 1.882\times10^{-3}T\ln T + 10.553\times10^{-6}T^2 - 9925.000T^{-1} + 24.887\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -157.364 - 133.825\times10^{-3}T + 51.580\times10^{-6}T^2 - 20535.500T^{-1}$

$\Delta Gf^\circ = -157.364 + 133.825\times10^{-3}T\ln T - 51.580\times10^{-6}T^2 - 10267.750T^{-1} - 894.747\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = -228.205 - 19.060\times10^{-3}T + 4.507\times10^{-6}T^2 - 20178.500T^{-1}$

$\Delta Gf^\circ = -228.205 + 19.060\times10^{-3}T\ln T - 4.507\times10^{-6}T^2 - 10089.250T^{-1} - 78.624\times10^{-3}T$

1667-1800 K: $\Delta Hf^\circ = -476.890 + 126.431\times10^{-3}T - 24.386\times10^{-6}T^2 + 122919.100T^{-1}$

$\Delta Gf^\circ = -476.890 - 126.431\times10^{-3}T\ln T + 24.386\times10^{-6}T^2 + 61459.550T^{-1} + 1076.010\times10^{-3}T$

Sources: Enthalpy of formation from Wagman (237). Low-temperature heat capacities and entropy 298 K from Westrum (247). High-temperature data based on Coughlin (43) corrected to IPTS-68 and Gronvold (86) whose data were given in IPTS-68.

Ga(c,l)

Gallium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.250	9.758	9.758	0
300	6.370	9.797	9.758	.012
302.9	6.540	9.858	9.758	.031
302.9	6.810	14.269	9.758	1.367
400	6.490	16.105	11.087	2.007
500	6.410	17.544	12.242	2.651
600	6.380	18.709	13.226	3.290
700	6.350	19.690	14.081	3.926
800	6.350	20.538	14.837	4.561
900	6.350	21.286	15.513	5.196
1000*	6.350	21.955	16.124	5.831
1100	6.350	22.560	16.682	6.466
1200	6.350	23.112	17.194	7.101
1300	6.350	23.621	17.670	7.736
1400	6.350	24.091	18.112	8.371
1500	6.350	24.529	18.525	9.006
1600	6.350	24.939	18.913	9.641
1700	6.350	25.324	19.279	10.276
1800	6.350	25.687	19.625	10.911
1900	6.350	26.030	19.953	11.546
2000	6.350	26.356	20.266	12.181

*Data extrapolated above 900 K.

Phase changes: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.
2478 K, boiling point of Ga; ΔH° = 61.8 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-302.9 K:

$$Cp^\circ = 6.496 + 0.200\times10^{-3}T$$

$$H^\circ - H^\circ_{298} = 6.496\times10^{-3}T + 0.100\times10^{-6}T^2 - 1.946$$

302.9-2000 K:

$$Cp^\circ = 6.000 + 0.252\times10^{-3}T + 0.672\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 6.000\times10^{-3}T + 0.126\times10^{-6}T^2 - 0.672\times10^{2}T^{-1} - 0.240$$

Source: Data from Hultgren (99) who extrapolated above 900 K by assuming constant heat capacity.

Ga(g)

Gallium (ideal monatomic gas)

[Formation: Ga(c,l) = Ga(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	6.058	40.375	40.375	0	66.200	57.072	-41.834
300	6.069	40.413	40.376	.011	66.199	57.014	-41.534
302.9	6.080	40.471	40.377	.029	66.198	56.925	-41.072
302.9	6.080	40.471	40.377	.029	64.862	56.925	-41.072
400	6.447	42.222	40.619	.641	64.834	54.387	-29.715
500	6.451	43.666	41.090	1.288	64.837	51.776	-22.631
600	6.290	44.829	41.619	1.926	64.836	49.164	-17.908
700	6.092	45.784	42.148	2.545	64.819	46.553	-14.534
800	5.909	46.585	42.654	3.145	64.784	43.946	-12.005
900	5.755	47.272	43.130	3.728	64.732	41.345	-10.040
1000	5.629	47.871	43.574	4.297	64.666	38.750	-8.469
1100	5.527	48.403	43.990	4.854	64.588	36.161	-7.184
1200	5.445	48.880	44.378	5.403	64.502	33.580	-6.116
1300	5.378	49.313	44.741	5.944	64.408	31.008	-5.213
1400	5.324	49.710	45.082	6.479	64.308	28.441	-4.440
1500	5.279	50.075	45.402	7.009	64.203	25.884	-3.771
1600	5.242	50.415	45.706	7.535	64.094	23.332	-3.187
1700	5.211	50.732	45.993	8.057	63.981	20.787	-2.672
1800	5.185	51.029	46.264	8.577	63.866	18.250	-2.216
1900	5.162	51.308	46.522	9.094	63.748	15.720	-1.808
2000	5.143	51.573	46.768	9.610	63.629	13.195	-1.442

Phase change: 302.9 K, melting point of Ga; $\Delta H° = 1.336$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.292 - 1.378\times10^{-3}T - 0.732\times10^{5}T^{-2}$

$H°- H°_{298} = 7.292\times10^{-3}T - 0.689\times10^{-6}T^{2} + 0.732\times10^{2}T^{-1} - 2.358$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf° = 65.787 + 0.796\times10^{-3}T - 0.789\times10^{-6}T^{2} + 73.200T^{-1}$

$\Delta Gf° = 65.787 - 0.796\times10^{-3}T\ln T + 0.789\times10^{-6}T^{2} + 36.600T^{-1} - 25.344\times10^{-3}T$

302.9-2000 K: $\Delta Hf° = 64.082 + 1.292\times10^{-3}T - 0.815\times10^{-6}T^{2} + 140.400T^{-1}$

$\Delta Gf° = 64.082 - 1.292\times10^{-3}T\ln T + 0.815\times10^{-6}T^{2} + 70.200T^{-1} - 17.253\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from Hilsenrath (94).

$Ga_2O_3(\beta)$

Digallium Trioxide, Gallium Sesquioxide

[Formation: $2Ga(c,l) + 1.5O_2(g) = Ga_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	22.020	20.310	20.310	0	-260.300	-238.620	174.911
300	22.086	20.446	20.310	.041	-260.302	-238.486	173.735
302.9	22.160	20.659	20.312	.105	-260.307	-238.276	171.920
302.9	22.160	20.659	20.312	.105	-262.979	-238.276	171.920
400	24.650	27.180	21.210	2.388	-263.010	-230.344	125.853
500	26.357	32.874	22.988	4.943	-262.840	-222.192	97.119
600	27.626	37.797	25.055	7.645	-262.548	-214.089	77.981
700	28.579	42.131	27.192	10.457	-262.175	-206.040	64.328
800	29.285	45.996	29.306	13.352	-261.747	-198.051	54.104
900	29.802	49.477	31.357	16.308	-261.283	-190.116	46.166
1000	30.182	52.637	33.329	19.308	-260.793	-182.235	39.827
1100	30.470	55.528	35.217	22.342	-260.288	-174.403	34.650
1200	30.703	58.190	37.023	25.400	-259.771	-166.620	30.345
1300	30.912	60.655	38.747	28.481	-259.244	-158.876	26.709
1400	31.116	62.954	40.395	31.583	-258.708	-151.178	23.600
1500	31.326	65.108	41.971	34.705	-258.161	-143.517	20.910
1600	31.544	67.136	43.481	37.848	-257.604	-135.891	18.562
1700	31.763	69.055	44.929	41.014	-257.031	-128.300	16.494
1800	31.965	70.877	46.321	44.200	-256.447	-120.745	14.660
1900	32.121	72.609	47.659	47.405	-255.853	-113.223	13.023
2000	32.196	74.259	48.948	50.622	-255.255	-105.730	11.554

Phase change: 302.9 K, melting point of Ga; $\Delta H° = 1.336$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 27.135 + 3.144\times10^{-3}T - 5.380\times10^{5}T^{-2}$

$H°- H°_{298} = 27.135\times10^{-3}T + 1.572\times10^{-6}T^{2} + 5.380\times10^{2}T^{-1} - 10.035$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf° = -262.915 + 3.298\times10^{-3}T + 0.617\times10^{-6}T^{2} + 470.200T^{-1}$

$\Delta Gf° = -262.915 - 3.298\times10^{-3}T\ln T - 0.617\times10^{-6}T^{2} + 235.100T^{-1} + 97.815\times10^{-3}T$

302.9-2000 K: $\Delta Hf° = -266.327 + 4.290\times10^{-3}T + 0.565\times10^{-6}T^{2} + 604.600T^{-1}$

$\Delta Gf° = -266.327 - 4.290\times10^{-3}T\ln T - 0.565\times10^{-6}T^{2} + 302.300T^{-1} + 113.997\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities and entropy at 298 K from King (128). High-temperature data based on Pankratz (175) corrected to IPTS-68.

Gd(c,l)

Gadolinium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	8.860	16.240	16.240	0
300	8.820	16.290	16.240	.016
400	6.730	18.410	16.528	.753
500	6.750	19.910	17.058	1.426
600	6.960	21.180	17.660	2.112
700	7.170	22.270	18.244	2.818
800	7.380	23.240	18.809	3.545
900	7.560	24.120	19.351	4.292
1000	7.770	24.920	19.861	5.059
1100	8.000	25.680	20.365	5.846
1200	8.250	26.380	20.832	6.658
1300	8.520	27.050	21.284	7.496
1400	8.820	27.700	21.726	8.363
1500	9.140	28.320	22.147	9.260
1533	9.250	28.520	22.281	9.565
1533	6.830	29.130	22.281	10.500
1585	6.830	29.350	22.503	10.855
1585	8.880	30.870	22.503	13.258
1600	8.880	30.950	22.581	13.391
1700	8.880	31.490	23.091	14.279
1800	8.880	32.000	23.574	15.167
1900	8.880	32.480	24.030	16.055
2000	8.880	32.930	24.458	16.943

Phase changes: 291.8 K, Curie temperature of Gd; $\Delta H^\circ = 0$
1533 K, $\alpha - \beta$ transition point of Gd; $\Delta H^\circ = 0.935$ kcal/mol.
1585 K, melting point of Gd; $\Delta H^\circ = 2.403$ kcal/mol.
3540 K, boiling point of Gd; $\Delta H^\circ = 85.9$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1533 K: $Cp^\circ = 2.786 + 4.406\times10^{-3}T + 4.231\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 2.786\times10^{-3}T + 2.203\times10^{-6}T^2 - 4.231\times10^{2}T^{-1} + 0.393$

1533-1585 K: $Cp^\circ = 6.827$

$H^\circ - H^\circ_{298} = 6.827\times10^{-3}T + 0.034$

1585-2000 K: $Cp^\circ = 8.880$

$H^\circ - H^\circ_{298} = 8.880\times10^{-3}T - 0.817$

Source: Data from Hultgren (99).

Gd(g)

Gadolinium (ideal monatomic gas)

[Formation: Gd(c,l) = Gd(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	6.584	46.416	46.416	0	95.000	86.003	-63.041
300	6.584	46.456	46.416	.012	94.996	85.946	-62.611
400	6.522	48.343	46.673	.668	94.915	82.942	-45.317
500	6.431	49.789	47.157	1.316	94.890	79.950	-34.946
600	6.319	50.952	47.697	1.953	94.841	76.978	-28.039
700	6.197	51.916	48.232	2.579	94.761	74.009	-23.106
800	6.079	52.736	48.745	3.193	94.648	71.051	-19.410
900	5.973	53.446	49.229	3.795	94.503	68.110	-16.539
1000	5.887	54.070	49.682	4.388	94.329	65.179	-14.245
1100	5.827	54.629	50.108	4.973	94.127	62.283	-12.374
1200	5.793	55.134	50.506	5.554	93.896	59.391	-10.816
1300	5.788	55.597	50.879	6.133	93.637	56.526	-9.503
1400	5.810	56.027	51.232	6.713	93.350	53.692	-8.382
1500	5.856	56.429	51.565	7.296	93.036	50.872	-7.412
1533	5.878	56.557	51.671	7.490	92.925	49.944	-7.120
1533	5.878	56.557	51.671	7.490	91.990	49.944	-7.120
1585	5.913	56.753	51.834	7.796	91.941	48.510	-6.689
1585	5.913	56.753	51.834	7.796	89.538	48.510	-6.689
1600	5.923	56.809	51.881	7.885	89.494	48.120	-6.573
1700	6.008	57.171	52.182	8.481	89.202	45.544	-5.855
1800	6.108	57.517	52.469	9.087	88.920	42.989	-5.220
1900	6.218	57.850	52.743	9.703	88.648	40.445	-4.652
2000	6.337	58.172	53.007	10.331	88.388	37.904	-4.142

Phase changes: 1533 K, α - β transition point of Gd; $\Delta H° = 0.935$ kcal/mol.
1585 K, melting point of Gd; $\Delta H° = 2.403$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.273 - 0.252\times10^{-3}T + 0.343\times10^{5}T^{-2}$

$H°-H°_{298} = 6.273\times10^{-3}T - 0.126\times10^{-6}T^{2} - 0.343\times10^{2}T^{-1} - 1.744$

Formation equations (kcal/mol):

298.15-1533 K: $\Delta Hf° = 92.863 + 3.487\times10^{-3}T - 2.329\times10^{-6}T^{2} + 388.800T^{-1}$

$\Delta Gf° = 92.863 - 3.487\times10^{-3}T\ln T + 2.329\times10^{-6}T^{2} + 194.400T^{-1} - 6.023\times10^{-3}T$

1533-1585 K: $\Delta Hf° = 93.222 - 0.554\times10^{-3}T - 0.126\times10^{-6}T^{2} - 34.300T^{-1}$

$\Delta Gf° = 93.222 + 0.554\times10^{-3}T\ln T + 0.126\times10^{-6}T^{2} - 17.150T^{-1} - 32.431\times10^{-3}T$

1585-2000 K: $\Delta Hf° = 94.073 - 2.607\times10^{-3}T - 0.126\times10^{-6}T^{2} - 34.300T^{-1}$

$\Delta Gf° = 94.073 + 2.607\times10^{-3}T\ln T + 0.126\times10^{-6}T^{2} - 17.150T^{-1} - 48.095\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). All other data from Feber (58).

Gd_2O_3(cubic)

Digadolinium Trioxide, Gadolinium Sesquioxide

[Formation: $2Gd(c) + 1.5O_2(g) = Gd_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	25.220	36.000	36.000	0	-436.640	-415.773	304.766
300	25.275	36.156	36.000	.047	-436.645	-415.645	302.793
400	27.359	43.751	37.021	2.692	-436.539	-408.657	223.277
500	28.503	49.989	39.011	5.489	-436.184	-401.728	175.593
600	29.291	55.259	41.291	8.381	-435.797	-394.849	143.822
700	29.911	59.822	43.619	11.342	-435.415	-388.051	121.153
800	30.437	63.851	45.901	14.360	-435.048	-381.312	104.168
900	30.898	67.463	48.100	17.427	-434.696	-374.616	90.968
1000	31.305	70.740	50.202	20.538	-434.359	-367.974	80.420
1100	31.658	73.741	52.208	23.686	-434.044	-361.329	71.789
1200	31.956	76.509	54.119	26.868	-433.758	-354.746	64.607
1300	32.193	79.076	55.941	30.076	-433.510	-348.173	58.532
1400	32.360	81.469	57.680	33.304	-433.312	-341.597	53.325
1500	32.451	83.705	59.342	36.545	-433.170	-335.048	48.816
1533	32.460	84.411	59.873	37.616	-433.141	-332.892	47.458
1533	32.460	84.411	59.873	37.616	-435.011	-332.892	47.458
1550	32.464	84.769	60.144	38.168	-434.916	-331.760	46.778

*Enthalpy of formation at 298 K estimated.

Phase change: 1533 K, α - β transition of Gd; $\Delta H° = 0.935$ kcal/mol.
1550 K, cubic to monoclinic transition point above 1500 K. Monoclinic form metastable below 1550 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1550 K: $Cp° = 28.491 + 3.094\times10^{-3}T - 3.728\times10^{5}T^{-2}$

$H°- H°_{298} = 28.491\times10^{-3}T + 1.547\times10^{-6}T^{2} + 3.728\times10^{2}T^{-1} - 9.882$

Formation equations (kcal/mol):

298.15-1533 K: $\Delta Hf° = -443.780 + 12.074\times10^{-3}T - 3.614\times10^{-6}T^{2} + 1151.200T^{-1}$

$\Delta Gf° = -443.780 - 12.074\times10^{-3}T\ln T + 3.614\times10^{-6}T^{2} + 575.600T^{-1} + 155.175\times10^{-3}T$

1533-1550 K: $\Delta Hf° = -443.063 + 3.992\times10^{-3}T + 0.793\times10^{-6}T^{2} + 305.000T^{-1}$

$\Delta Gf° = -443.063 - 3.992\times10^{-3}T\ln T - 0.793\times10^{-6}T^{2} + 152.500T^{-1} + 102.360\times10^{-3}T$

Sources: Enthalpy of formation at 298 K estimated by Gschneidner (90). Low-temperature heat capacities and entropy at 298 K from Justice (110). High-temperature data based on Pankratz (179).

Gd_2O_3(monoclinic)

Digadolinium Trioxide, Gadolinium Sesquioxide

[Formation: $2Gd(c,l) + 1.5O_2(g) = Gd_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	25.484	37.500	37.500	0	-434.900	-414.480	303.818
300	25.524	37.658	37.501	.047	-434.905	-414.356	301.854
400	27.105	45.240	38.525	2.686	-434.805	-407.519	222.655
500	28.067	51.398	40.502	5.448	-434.485	-400.733	175.158
600	28.749	56.579	42.761	8.291	-434.147	-393.991	143.509
700	29.283	61.052	45.062	11.193	-433.824	-387.321	120.926
800	29.734	64.992	47.312	14.144	-433.523	-380.701	104.001
900	30.141	68.518	49.475	17.139	-433.243	-374.113	90.846
1000	30.527	71.714	51.542	20.172	-432.985	-367.574	80.332
1100	30.908	74.641	53.510	23.244	-432.746	-361.021	71.727
1200	31.292	77.347	55.385	26.354	-432.531	-354.525	64.567
1300	31.682	79.867	57.173	29.502	-432.343	-348.035	58.509
1400	32.076	82.230	58.880	32.690	-432.185	-341.536	53.316
1500	32.468	84.456	60.511	35.917	-432.057	-335.062	48.818
1533	32.593	85.164	61.034	36.991	-432.027	-332.932	47.463
1533	32.593	85.164	61.034	36.991	-433.897	-332.932	47.463
1585*	32.790	86.255	61.844	38.691	-433.592	-329.531	45.437
1585	32.790	86.255	61.844	38.691	-438.398	-329.531	45.437
1600	32.847	86.564	62.075	39.183	-438.369	-328.506	44.871
1700	33.199	88.566	63.574	42.486	-438.165	-321.638	41.349
1800	33.504	90.472	65.015	45.822	-437.937	-314.779	38.219
1900	33.739	92.290	66.403	49.185	-437.691	-307.945	35.421
2000	33.876	94.025	67.742	52.566	-437.434	-301.146	32.907

*Monoclinic form is metastable below 1550 K.

Phase changes: 1533 K, α - β transition point of Gd; $\Delta H°$ = 0.935 kcal/mol.
1585 K, melting point of Gd; $\Delta H°$ = 2.403 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 27.365 + 3.458\times10^{-3}T - 2.588\times10^{5}T^{-2}$

$H°- H°_{298} = 27.365\times10^{-3}T + 1.729\times10^{-6}T^{2} + 2.588\times10^{2}T^{-1} - 9.181$

Formation equations (kcal/mol):

298.15-1533 K: $\Delta Hf° = -441.338 + 10.948\times10^{-3}T - 3.432\times10^{-6}T^{2} + 1037.200T^{-1}$

$\Delta Gf° = -441.338 - 10.948\times10^{-3}T\ln T + 3.432\times10^{-6}T^{2} + 518.600T^{-1} + 145.601\times10^{-3}T$

1533-1585 K: $\Delta Hf° = -440.621 + 2.866\times10^{-3}T + 0.975\times10^{-6}T^{2} + 191.000T^{-1}$

$\Delta Gf° = -440.621 - 2.866\times10^{-3}T\ln T - 0.975\times10^{-6}T^{2} + 95.500T^{-1} + 92.786\times10^{-3}T$

1585-2000 K: $\Delta Hf° = -438.919 - 1.240\times10^{-3}T + 0.975\times10^{-6}T^{2} + 191.000T^{-1}$

$\Delta Gf° = -438.919 + 1.240\times10^{-3}T\ln T - 0.975\times10^{-6}T^{2} + 95.500T^{-1} + 61.458\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). Entropy at 298 K estimated using data from Hoekstra (95). High-temperature data based on Pankratz (179).

Ge(c,1)

Germanium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.580	7.430	7.430	0
300	5.580	7.460	7.430	.010
400	5.850	9.110	7.647	.585
500	5.950	10.430	8.080	1.175
600	6.030	11.530	8.572	1.775
700	6.100	12.460	9.057	2.382
800	6.190	13.280	9.535	2.996
900	6.330	14.020	9.996	3.622
1000	6.500	14.690	10.426	4.264
1100	6.680	15.320	10.845	4.923
1200	6.860	15.910	11.244	5.599
1210.4	6.870	15.970	11.288	5.670
1210.4	6.600	23.270	11.288	14.500
1300	6.600	23.740	12.132	15.090
1400	6.600	24.230	12.980	15.750
1500	6.600	24.690	13.750	16.410
1600*	6.600	25.110	14.441	17.070
1700	6.600	25.510	15.081	17.730
1800	6.600	25.890	15.673	18.390
1900	6.600	26.250	16.224	19.050
2000	6.600	26.590	16.735	19.710

*Data extrapolated above 1500 K.

Phase changes: 1210.4 K, melting point of Ge; ΔH° = 8.830 kcal/mol.
3107 K, boiling point of Ge; ΔH° = 79.1 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15–1210.4 K: $Cp^\circ = 5.581 + 0.932\times10^{-3}T - 0.249\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.581\times10^{-3}T + 0.466\times10^{-6}T^{2} + 0.249\times10^{2}T^{-1} - 1.789$

1210.4–2000 K: $Cp^\circ = 6.600$

$H^\circ - H^\circ_{298} = 6.600\times10^{-3}T + 6.511$

Source: Data from Hultgren (99) who extrapolated above 1500 K by assuming constant heat capacity.

Ge(g)

Germanium (ideal monatomic gas)

[Formation: Ge(c,1) = Ge(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.345	40.104	40.104	0	89.500	79.758	-58.464
300	7.351	40.149	40.104	.014	89.504	79.697	-58.059
400	7.426	42.283	40.393	.756	89.671	76.402	-41.743
500	7.256	43.925	40.943	1.491	89.816	73.068	-31.938
600	6.995	45.226	41.553	2.204	89.929	69.711	-25.392
700	6.716	46.283	42.156	2.889	90.007	66.331	-20.709
800	6.460	47.162	42.727	3.548	90.052	62.946	-17.196
900	6.240	47.910	43.262	4.183	90.061	59.560	-14.463
1000	6.059	48.558	43.761	4.797	90.033	56.165	-12.275
1100	5.913	49.128	44.223	5.396	89.973	52.784	-10.487
1200	5.799	49.638	44.654	5.981	89.882	49.408	-8.998
1210.4	5.790	49.688	44.697	6.041	89.871	49.062	-8.859
1210.4	5.790	49.688	44.697	6.041	81.041	49.062	-8.859
1300	5.712	50.098	45.055	6.556	80.966	46.701	-7.851
1400	5.646	50.519	45.430	7.124	80.874	44.069	-6.879
1500	5.599	50.907	45.783	7.686	80.776	41.450	-6.039
1600	5.566	51.267	46.114	8.244	80.674	38.823	-5.303
1700	5.544	51.604	46.428	8.800	80.570	36.210	-4.655
1800	5.531	51.920	46.724	9.353	80.463	33.609	-4.081
1900	5.525	52.219	47.005	9.906	80.356	31.015	-3.567
2000	5.524	52.503	47.273	10.459	80.249	28.423	-3.106

Phase change: 1210.4 K, melting point of Ge; $\Delta H° = 8.830$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.000 - 1.664\times10^{-3}T - 0.141\times10^{5}T^{-2}$

$H°- H°_{298} = 8.000\times10^{-3}T - 0.832\times10^{-6}T^{2} + 0.141\times10^{2}T^{-1} - 2.359$

Formation equations (kcal/mol):

298.15-1210.4 K: $\Delta Hf° = 88.930 + 2.419\times10^{-3}T - 1.298\times10^{-6}T^{2} - 10.800T^{-1}$

$\Delta Gf° = 88.930 - 2.419\times10^{-3}T\ln T + 1.298\times10^{-6}T^{2} - 5.400T^{-1} - 17.307\times10^{-3}T$

1210.4-2000 K: $\Delta Hf° = 80.630 + 1.400\times10^{-3}T - 0.832\times10^{-6}T^{2} + 14.100T^{-1}$

$\Delta Gf° = 80.630 - 1.400\times10^{-3}T\ln T + 0.832\times10^{-6}T^{2} + 7.050T^{-1} - 17.128\times10^{-3}T$

Sources: Enthalpy of formation from CODATA (37). All other data from Hilsenrath (94).

GeO_2(hexagonal)

Germanium Dioxide

[Formation: $Ge(c,l) + O_2(g) = GeO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.450	13.210	13.210	0	-132.580	-119.692	87.736
300	12.484	13.287	13.210	.023	-132.580	-119.613	87.137
400	14.006	17.100	13.720	1.352	-132.536	-115.296	62.994
500	15.119	20.351	14.729	2.811	-132.398	-110.998	48.517
600	15.964	23.185	15.907	4.367	-132.197	-106.732	38.877
700	16.606	25.697	17.130	5.997	-131.952	-102.511	32.005
800	17.089	27.947	18.343	7.683	-131.678	-98.324	26.860
900	17.446	29.982	19.525	9.411	-131.390	-94.169	22.867
1000	17.708	31.834	20.665	11.169	-131.101	-90.055	19.681
1100	17.906	33.532	21.759	12.950	-130.818	-85.962	17.079
1200	18.067	35.097	22.806	14.749	-130.543	-81.894	14.915
1210.4	18.083	35.253	22.912	14.937	-130.515	-81.468	14.710
1210.4	18.083	35.253	22.912	14.937	-139.345	-81.468	14.710
1300	18.220	36.549	23.808	16.563	-139.076	-77.191	12.977
1389	18.371	37.760	24.664	18.191	-138.804	-72.962	11.480

Phase changes: 1210.4 K, melting point of Ge; $\Delta H° = 8.830$ kcal/mol.
1389 K, melting point of GeO_2(hexagonal); $\Delta H° = 3 \pm 1$ kcal/mol. Conflicting data prevent further resolution. Hexagonal GeO_2 is metastable below 1308 K. On cooling, liquid solidifies to vitreous form.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1389 K: $Cp° = 14.623 + 3.296\times10^{-3}T - 2.805\times10^{5}T^{-2}$

$H°- H°_{298} = 14.623\times10^{-3}T + 1.648\times10^{-6}T^2 + 2.805\times10^{2}T^{-1} - 5.447$

Formation equations (kcal/mol):

298.15-1210.4 K: $\Delta Hf° = -133.886 + 1.812\times10^{-3}T + 0.679\times10^{-6}T^2 + 210.400T^{-1}$

$\Delta Gf° = -133.886 - 1.812\times10^{-3}T\ln T - 0.679\times10^{-6}T^2 + 105.200T^{-1} + 56.949\times10^{-3}T$

1210.4-1389 K: $\Delta Hf° = -142.186 + 0.793\times10^{-3}T + 1.145\times10^{-6}T^2 + 235.300T^{-1}$

$\Delta Gf° = -142.186 - 0.793\times10^{-3}T\ln T - 1.145\times10^{-6}T^2 + 117.650T^{-1} + 57.129\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Gross (88). Low-temperature heat capacities and entropy at 298 K from King (128). High-temperature data based on Kelley (121).

GeO_2(tetragonal)

Germanium Dioxide

[Formation: $Ge(c,l) + O_2(g) = GeO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	11.990	9.490	9.490	0	-138.600	-124.603	91.336
300	12.047	9.564	9.491	.022	-138.601	-124.517	90.710
400	14.424	13.401	9.998	1.361	-138.547	-119.827	65.470
500	15.758	16.775	11.023	2.876	-138.353	-115.165	50.338
600	16.572	19.726	12.233	4.496	-138.088	-110.547	40.266
700	17.091	22.323	13.493	6.181	-137.788	-105.985	33.090
800	17.458	24.630	14.744	7.909	-137.472	-101.464	27.718
900	17.769	26.704	15.960	9.670	-137.151	-96.979	23.550
1000	18.085	28.592	17.129	11.463	-136.827	-92.539	20.224
1100	18.436	30.332	18.251	13.289	-136.499	-88.123	17.508
1200	18.824	31.953	19.327	15.151	-136.161	-83.739	15.251
1210.4	18.866	32.116	19.436	15.347	-136.125	-83.282	15.037
1210.4	18.866	32.116	19.436	15.347	-144.955	-83.282	15.037
1300	19.224	33.475	20.357	17.054	-144.605	-78.724	13.234
1308	19.255	33.593	20.437	17.208	-144.573	-78.318	13.086

Phase changes: 1210.4 K, melting point of Ge; ΔH° = 8.830 kcal/mol.
1308 K, transition point to hexagonal form; ΔH° = 5 ± 1 kcal/mol. Conflicting data prevent further resolution. Hexagonal form metastable below 1308 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1308 K: $Cp^\circ = 16.457 + 2.178\times10^{-3}T - 4.549\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 16.457\times10^{-3}T + 1.089\times10^{-6}T^2 + 4.549\times10^{2}T^{-1} - 6.529$

Formation equations (kcal/mol):

298.15-1210.4 K: $\Delta Hf^\circ = -140.988 + 3.646\times10^{-3}T + 0.120\times10^{-6}T^2 + 384.800T^{-1}$

$\Delta Gf^\circ = -140.988 - 3.646\times10^{-3}T\ln T - 0.120\times10^{-6}T^2 + 192.400T^{-1} + 73.600\times10^{-3}T$

1210.4-1308 K: $\Delta Hf^\circ = -149.288 + 2.627\times10^{-3}T + 0.586\times10^{-6}T^2 + 409.700T^{-1}$

$\Delta Gf^\circ = -149.288 - 2.627\times10^{-3}T\ln T - 0.586\times10^{-6}T^2 + 204.850T^{-1} + 73.779\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Gross (88). Low-temperature heat capacities and entropy at 298 K from Counsell (44). High-temperature data based on Andon (8) and Tsagareishvili (227).

GeO_2(vitreous)

Germanium Dioxide

[Formation: $Ge(c,1) + O_2(g) = GeO_2(vit)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.667	15.420	15.420	0	-128.400	-116.171	85.155
300	12.706	15.498	15.421	.023	-128.400	-116.097	84.575
400	14.250	19.375	15.938	1.375	-128.333	-112.003	61.195
500	15.317	22.676	16.964	2.856	-128.173	-107.935	47.178
600	16.115	25.542	18.160	4.429	-127.955	-103.904	37.847
700	16.743	28.075	19.398	6.074	-127.695	-99.918	31.195
800	17.246	30.345	20.628	7.774	-127.407	-95.971	26.218
900	17.654	32.401	21.823	9.520	-127.101	-92.057	22.354
1000	17.985	34.279	22.977	11.302	-126.788	-88.187	19.273
1100	18.255	36.006	24.083	13.115	-126.473	-84.339	16.756
1200	18.478	37.604	25.144	14.952	-126.160	-80.519	14.664
1210.4	18.497	37.764	25.252	15.144	-126.127	-80.120	14.466
1210.4	18.497	37.764	25.252	15.144	-134.957	-80.120	14.466
1300	18.665	39.091	26.161	16.809	-134.650	-76.069	12.788
1400	18.829	40.480	27.134	18.684	-134.299	-71.575	11.173
1500	18.981	41.784	28.068	20.574	-133.939	-67.100	9.776
1600	19.130	43.014	28.964	22.480	-133.570	-62.666	8.560
1700	19.289	44.179	29.825	24.401	-133.191	-58.246	7.488
1800	19.467	45.286	30.654	26.338	-132.802	-53.843	6.537

Phase change: 1210.4 K, melting point of Ge; $\Delta H° = 8.830$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 15.156 + 2.882\times10^{-3}T - 2.976\times10^{5}T^{-2}$

$H°- H°_{298} = 15.156\times10^{-3}T + 1.441\times10^{-6}T^{2} + 2.976\times10^{2}T^{-1} - 5.645$

Formation equations (kcal/mol):

298.15-1210.4 K: $\Delta Hf° = -129.904 + 2.345\times10^{-3}T + 0.472\times10^{-6}T^{2} + 227.500T^{-1}$

$\Delta Gf° = -129.904 - 2.345\times10^{-3}T\ln T - 0.472\times10^{-6}T^{2} + 113.750T^{-1} + 58.282\times10^{-3}T$

1210.4-1800 K: $\Delta Hf° = -138.204 + 1.326\times10^{-3}T + 0.938\times10^{-6}T^{2} + 252.400T^{-1}$

$\Delta Gf° = -138.204 - 1.326\times10^{-3}T\ln T - 0.938\times10^{-6}T^{2} + 126.200T^{-1} + 58.461\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Entropy at 298 K from Mah (149). Low-temperature heat capacities from Tarasov (217). High-temperature data based on Kelley (121).

$H_2(g)$

Hydrogen

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.892	31.207	31.207	0
300	6.895	31.250	31.207	.013
400	6.974	33.247	31.480	.707
500	6.993	34.806	31.994	1.406
600	7.009	36.082	32.572	2.106
700	7.036	37.164	33.153	2.808
800	7.080	38.107	33.715	3.514
900	7.142	38.944	34.250	4.225
1000	7.219	39.700	34.757	4.943
1100	7.309	40.392	35.238	5.669
1200	7.407	41.033	35.695	6.405
1300	7.510	41.630	36.129	7.151
1400	7.615	42.190	36.542	7.907
1500	7.719	42.719	36.936	8.674
1600	7.821	43.220	37.313	9.451
1700	7.920	43.698	37.676	10.238
1800	8.016	44.153	38.022	11.035
1900	8.106	44.589	38.357	11.841
2000	8.193	45.007	38.679	12.656
2100	8.275	45.409	38.990	13.479
2200	8.354	45.795	39.290	14.311
2300	8.428	46.168	39.581	15.150
2400	8.499	46.529	39.864	15.996
2500	8.566	46.877	40.137	16.849
2600	8.631	47.214	40.403	17.709
2700	8.692	47.541	40.661	18.575
2800	8.752	47.858	40.912	19.448
2900	8.809	48.166	41.157	20.326
3000	8.864	48.466	41.396	21.209

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 6.456 + 0.838\times10^{-3}T + 0.165\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.456\times10^{-3}T + 0.419\times10^{-6}T^{2} - 0.165\times10^{2}T^{-1} - 1.907$

Source: Data from JANAF (52).

H(g)

Hydrogen (ideal monatomic gas)

[Formation: $0.5H_2(g) = H(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	27.392	27.392	0	52.103	48.588	-35.616
300	4.968	27.422	27.392	.009	52.105	48.566	-35.380
400	4.968	28.852	27.587	.506	52.256	47.364	-25.878
500	4.968	29.960	27.954	1.003	52.403	46.125	-20.161
600	4.968	30.866	28.366	1.500	52.550	44.855	-16.338
700	4.968	31.632	28.781	1.996	52.695	43.560	-13.600
800	4.968	32.295	29.179	2.493	52.839	42.246	-11.541
900	4.968	32.880	29.558	2.990	52.981	40.913	-9.935
1000	4.968	33.404	29.917	3.487	53.118	39.565	-8.647
1100	4.968	33.877	30.255	3.984	53.253	38.203	-7.590
1200	4.968	34.309	30.576	4.480	53.381	36.830	-6.707
1300	4.968	34.707	30.879	4.977	53.505	35.445	-5.959
1400	4.968	35.075	31.165	5.474	53.624	34.051	-5.316
1500	4.968	35.418	31.437	5.971	53.737	32.649	-4.757
1600	4.968	35.739	31.696	6.468	53.846	31.239	-4.267
1700	4.968	36.040	31.944	6.964	53.948	29.823	-3.834
1800	4.968	36.324	32.179	7.461	54.047	28.401	-3.448
1900	4.968	36.592	32.404	7.958	54.141	26.975	-3.103
2000	4.968	36.847	32.619	8.455	54.230	25.543	-2.791
2100	4.968	37.090	32.827	8.952	54.316	24.106	-2.509
2200	4.968	37.321	33.026	9.448	54.396	22.664	-2.251
2300	4.968	37.542	33.218	9.945	54.473	21.220	-2.016
2400	4.968	37.753	33.402	10.442	54.547	19.775	-1.801
2500	4.968	37.956	33.580	10.939	54.618	18.324	-1.602
2600	4.968	38.151	33.753	11.436	54.685	16.870	-1.418
2700	4.968	38.338	33.919	11.932	54.748	15.415	-1.248
2800	4.968	38.519	34.080	12.429	54.808	13.956	-1.089
2900	4.968	38.693	34.236	12.926	54.866	12.497	-.942
3000	4.968	38.862	34.388	13.423	54.922	11.035	-.804

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 4.968$

$H°- H°_{298} = 4.968\times10^{-3}T - 1.481$

Formation equations (kcal/mol):

298.15-3000 K: $\Delta Hf° = 51.575 + 1.740\times10^{-3}T - 0.209\times10^{-6}T^2 + 8.250T^{-1}$

$\Delta Gf° = 51.575 - 1.740\times10^{-3}T\ln T + 0.209\times10^{-6}T^2 + 4.125T^{-1} - 0.213\times10^{-3}T$

Source: Data from JANAF (52).

$D_2(g)$

Deuterium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.978	34.620	34.620	0
300	6.978	34.663	34.620	.013
400	6.989	36.672	34.895	.711
500	7.019	38.234	35.412	1.411
600	7.079	39.519	35.992	2.116
700	7.172	40.616	36.576	2.828
800	7.290	41.582	37.143	3.551
900	7.423	42.448	37.685	4.287
1000	7.561	43.237	38.201	5.036
1100	7.698	43.964	38.692	5.799
1200	7.830	44.640	39.161	6.575
1300	7.954	45.272	39.607	7.365
1400	8.070	45.865	40.032	8.166
1500	8.177	46.426	40.440	8.979
1600	8.275	46.957	40.831	9.801
1700	8.366	47.461	41.206	10.633
1800	8.450	47.942	41.568	11.474
1900	8.527	48.401	41.915	12.323
2000	8.598	48.840	42.250	13.179

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 6.264 + 1.258\times10^{-3}T + 0.301\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.264\times10^{-3}T + 0.629\times10^{-6}T^2 - 0.301\times10^{2}T^{-1} - 1.823$

Source: Data from JANAF (52).

D(g)

Deuterium (ideal monatomic gas)

[Formation: $0.5D_2(g) = D(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	4.968	29.455	29.455	0	52.992	49.371	-36.189
300	4.968	29.486	29.456	.009	52.994	49.348	-35.950
400	4.968	30.915	29.650	.506	53.143	48.111	-26.286
500	4.968	32.024	30.018	1.003	53.289	46.836	-20.472
600	4.968	32.930	30.430	1.500	53.434	45.532	-16.585
700	4.968	33.695	30.844	1.996	53.574	44.203	-13.801
800	4.968	34.359	31.243	2.493	53.709	42.855	-11.707
900	4.968	34.944	31.622	2.990	53.839	41.491	-10.075
1000	4.968	35.467	31.980	3.487	53.961	40.112	-8.766
1100	4.968	35.941	32.319	3.984	54.077	38.722	-7.693
1200	4.968	36.373	32.640	4.480	54.185	37.321	-6.797
1300	4.968	36.771	32.943	4.977	54.287	35.911	-6.037
1400	4.968	37.139	33.229	5.474	54.383	34.494	-5.385
1500	4.968	37.482	33.501	5.971	54.474	33.070	-4.818
1600	4.968	37.802	33.759	6.468	54.559	31.642	-4.322
1700	4.968	38.103	34.007	6.964	54.639	30.206	-3.883
1800	4.968	38.387	34.242	7.461	54.716	28.767	-3.493
1900	4.968	38.656	34.468	7.958	54.789	27.323	-3.143
2000	4.968	38.911	34.683	8.455	54.858	25.876	-2.828

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.968$

$H°- H°_{298} = 4.968\times10^{-3}T - 1.481$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 52.422 + 1.836\times10^{-3}T - 0.315\times10^{-6}T^2 + 15.050T^{-1}$

$\Delta Gf° = 52.422 - 1.836\times10^{-3}T\ln T + 0.315\times10^{-6}T^2 + 7.525T^{-1} + 0.049\times10^{-3}T$

Source: Data from JANAF (52).

OH(g)

Hydroxyl (ideal gas)

[Formation: $0.5H_2(g) + 0.5O_2(g) = OH(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.167	43.881	43.881	0	9.318	8.192	-6.005
300	7.165	43.926	43.883	.013	9.318	8.185	-5.963
400	7.087	45.974	44.161	.725	9.328	7.806	-4.265
500	7.056	47.552	44.688	1.432	9.320	7.426	-3.246
600	7.057	48.838	45.276	2.137	9.297	7.048	-2.567
700	7.090	49.928	45.864	2.845	9.266	6.677	-2.085
800	7.150	50.878	46.433	3.556	9.224	6.309	-1.723
900	7.233	51.725	46.975	4.275	9.181	5.947	-1.444
1000	7.332	52.492	47.488	5.004	9.138	5.590	-1.222
1100	7.439	53.196	47.976	5.742	9.093	5.238	-1.041
1200	7.549	53.848	48.439	6.491	9.050	4.889	-.890
1300	7.659	54.456	48.878	7.252	9.010	4.545	-.764
1400	7.766	55.028	49.297	8.023	8.971	4.202	-.656
1500	7.867	55.567	49.697	8.805	8.935	3.863	-.563
1600	7.963	56.078	50.080	9.596	8.898	3.525	-.481
1700	8.053	56.564	50.448	10.397	8.865	3.190	-.410
1800	8.137	57.026	50.800	11.207	8.832	2.859	-.347
1900	8.214	57.468	51.140	12.024	8.800	2.528	-.291
2000	8.286	57.891	51.466	12.849	8.767	2.199	-.240
2100	8.353	58.297	51.782	13.682	8.736	1.873	-.195
2200	8.415	58.687	52.087	14.520	8.704	1.545	-.153
2300	8.473	59.063	52.383	15.364	8.670	1.218	-.116
2400	8.526	59.425	52.669	16.214	8.637	.895	-.082
2500	8.576	59.774	52.946	17.069	8.602	.573	-.050
2600	8.622	60.111	53.215	17.929	8.567	.253	-.021
2700	8.665	60.437	53.476	18.794	8.531	-.065	.005
2800	8.706	60.753	53.731	19.662	8.492	-.383	.030
2900	8.744	61.059	53.978	20.535	8.452	-.698	.053
3000	8.780	61.356	54.219	21.411	8.411	-1.013	.074

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 6.357 + 0.952\times10^{-3}T + 0.468\times10^{5}T^{-2}$

$H°- H°_{298} = 6.357\times10^{-3}T + 0.476\times10^{-6}T^{2} - 0.468\times10^{2}T^{-1} - 1.781$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 9.667 - 0.486\times10^{-3}T + 0.015\times10^{-6}T^{2} - 61.150T^{-1}$

$\Delta Gf° = 9.667 + 0.486\times10^{-3}T\ln T - 0.015\times10^{-6}T^{2} - 30.575T^{-1} - 7.365\times10^{-3}T$

2000-3000 K: $\Delta Hf° = 10.335 - 1.041\times10^{-3}T + 0.162\times10^{-6}T^{2} - 353.550T^{-1}$

$\Delta Gf° = 10.335 + 1.041\times10^{-3}T\ln T - 0.162\times10^{-6}T^{2} - 176.775T^{-1} - 11.587\times10^{-3}T$

Source: Data from JANAF (53).

$HO_2(g)$

Hydroperoxyl (ideal gas)

[Formation: $0.5H_2(g) + O_2(g) = HO_2(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.343	54.731	54.731	0	0.500	3.445	-2.525
300	8.352	54.783	54.733	.015	.495	3.463	-2.523
400	8.914	57.260	55.065	.878	.301	4.483	-2.449
500	9.485	59.312	55.716	1.798	.141	5.547	-2.425
600	9.986	61.087	56.465	2.773	.011	6.642	-2.419
700	10.411	62.659	57.240	3.793	-.098	7.755	-2.421
800	10.775	64.073	58.007	4.853	-.189	8.883	-2.427
900	11.094	65.361	58.753	5.947	-.265	10.023	-2.434
1000	11.378	66.545	59.475	7.070	-.327	11.168	-2.441
1100	11.633	67.642	60.168	8.221	-.378	12.320	-2.448
1200	11.865	68.664	60.834	9.396	-.420	13.477	-2.454
1300	12.078	69.622	61.473	10.594	-.451	14.637	-2.461
1400	12.275	70.525	62.089	11.811	-.476	15.797	-2.466
1500	12.459	71.378	62.679	13.048	-.492	16.960	-2.471
1600	12.630	72.187	63.248	14.303	-.502	18.125	-2.476
1700	12.791	72.958	63.797	15.574	-.507	19.290	-2.480
1800	12.942	73.693	64.326	16.861	-.507	20.455	-2.484
1900	13.084	74.397	64.838	18.162	-.503	21.618	-2.487
2000	13.217	75.072	65.333	19.477	-.494	22.781	-2.489

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations::

298.15-2000 K: $Cp° = 8.880 + 2.416\times10^{-3}T - 1.118\times10^{5}T^{-2}$

$H°- H°_{298} = 8.880\times10^{-3}T + 1.208\times10^{-6}T^{2} + 1.118\times10^{2}T^{-1} - 3.130$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 0.675 - 1.578\times10^{-3}T + 0.495\times10^{-6}T^{2} + 74.850T^{-1}$

$\Delta Gf° = 0.675 + 1.578\times10^{-3}T\ln T - 0.495\times10^{-6}T^{2} + 37.425T^{-1} + 0.025\times10^{-3}T$

Source: Data from JANAF (56).

$H_2O(l,g)$

Water

[Formation: $H_2(g) + 0.5O_2(g) = H_2O(l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.997	16.718	16.718	0	-68.315	-56.690	41.554
300	17.995	16.829	16.719	.033	-68.302	-56.618	41.246
373.15	18.153	20.765	17.139	1.353	-67.747	-53.831	31.528
373.15	8.134	46.921	17.139	11.113	-57.987	-53.831	31.528
400	8.186	47.484	19.124	11.344	-58.040	-53.516	29.240
500	8.415	49.334	24.988	12.173	-58.275	-52.359	22.886
600	8.676	50.891	29.178	13.028	-58.498	-51.154	18.633
700	8.954	52.249	32.379	13.909	-58.708	-49.913	15.583
800	9.246	53.464	34.940	14.819	-58.903	-48.644	13.289
900	9.547	54.570	37.060	15.759	-59.081	-47.350	11.498
1000	9.851	55.592	38.864	16.728	-59.243	-46.040	10.062
1100	10.152	56.545	40.428	17.729	-59.388	-44.711	8.883
1200	10.444	57.441	41.809	18.759	-59.518	-43.370	7.899
1300	10.723	58.288	43.044	19.817	-59.634	-42.020	7.064
1400	10.987	59.092	44.161	20.903	-59.736	-40.661	6.347
1500	11.233	59.859	45.183	22.014	-59.827	-39.297	5.725
1600	11.462	60.591	46.123	23.149	-59.907	-37.925	5.180
1700	11.674	61.293	46.995	24.306	-59.978	-36.549	4.699
1800	11.869	61.965	47.808	25.483	-60.042	-35.168	4.270
1900	12.048	62.612	48.570	26.679	-60.099	-33.785	3.886
2000	12.214	63.234	49.288	27.892	-60.151	-32.399	3.540
2100	12.366	63.834	49.967	29.121	-60.197	-31.009	3.227
2200	12.505	64.412	50.610	30.365	-60.240	-29.619	2.942
2300	12.634	64.971	51.222	31.622	-60.280	-28.227	2.682
2400	12.753	65.511	51.806	32.891	-60.318	-26.830	2.443
2500	12.863	66.034	52.365	34.172	-60.353	-25.435	2.223
2600	12.965	66.541	52.901	35.464	-60.386	-24.039	2.021
2700	13.059	67.032	53.415	36.765	-60.419	-22.641	1.833
2800	13.146	67.508	53.910	38.075	-60.453	-21.240	1.658
2900	13.228	67.971	54.387	39.394	-60.485	-19.840	1.495
3000	13.304	68.421	54.848	40.720	-60.517	-18.437	1.343

Phase changes: 273.15 K, melting point of H_2O; $\Delta H°$ = 1.436 kcal/mol.
373.15 K, boiling point of H_2O; $\Delta H°$ = 9.760 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-373.15 K: $Cp° = 18.041$

$H°- H°_{298} = 18.041 \times 10^{-3} T - 5.379$

373.15-3000 K: $Cp° = 7.272 + 2.492 \times 10^{-3} T - 0.094 \times 10^{5} T^{-2}$

$H°- H°_{298} = 7.272 \times 10^{-3} T + 1.246 \times 10^{-6} T^{2} + 0.094 \times 10^{2} T^{-1} + 8.201$

$H_2O(l,g)$ - Continued

Formation equations (kcal/mol):

298.15-373.15 K: $\Delta Hf° = -70.611 + 7.970x10^{-3}T - 0.671x10^{-6}T^2 - 6.100T^{-1}$

$\Delta Gf° = -70.611 - 7.970x10^{-3}TlnT + 0.671x10^{-6}T^2 - 3.050T^{-1} + 91.937x10^{-3}T$

373.15-2000 K: $\Delta Hf° = -57.031 - 2.799x10^{-3}T + 0.576x10^{-6}T^2 + 3.300T^{-1}$

$\Delta Gf° = -57.031 + 2.799x10^{-3}TlnT - 0.576x10^{-6}T^2 + 1.650T^{-1} - 7.798x10^{-3}T$

2000-3000 K: $\Delta Hf° = -56.363 - 3.354x10^{-3}T + 0.722x10^{-6}T^2 - 289.100T^{-1}$

$\Delta Gf° = -56.363 + 3.354x10^{-3}TlnT - 0.722x10^{-6}T^2 - 144.550T^{-1} - 12.020x10^{-3}T$

Sources: Enthalpy of formation at 298 K for liquid and gas from CODATA (36). Entropy at 298 K for liquid also from CODATA (36). Data for liquid from Ginnings (77). Data for gas from JANAF (51).

$H_2O(g)$

Water (ideal gas)

[Formation: $H_2(g) + 0.5O_2(g) = H_2O(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.025	45.106	45.106	0	-57.795	-54.634	40.047
300	8.027	45.155	45.106	.015	-57.799	-54.614	39.786
400	8.186	47.484	45.422	.825	-58.038	-53.515	29.239
500	8.415	49.334	46.026	1.654	-58.274	-52.358	22.885
600	8.676	50.891	46.709	2.509	-58.496	-51.153	18.632
700	8.954	52.249	47.406	3.390	-58.707	-49.912	15.583
800	9.246	53.464	48.089	4.300	-58.902	-48.643	13.289
900	9.547	54.570	48.748	5.240	-59.080	-47.349	11.498
1000	9.851	55.592	49.383	6.209	-59.242	-46.039	10.062
1100	10.152	56.545	49.990	7.210	-59.387	-44.710	8.883
1200	10.444	57.441	50.574	8.240	-59.517	-43.369	7.899
1300	10.723	58.288	51.136	9.298	-59.632	-42.019	7.064
1400	10.987	59.092	51.675	10.384	-59.735	-40.660	6.347
1500	11.233	59.859	52.196	11.495	-59.826	-39.296	5.725
1600	11.462	60.591	52.697	12.630	-59.906	-37.924	5.180
1700	11.674	61.293	53.183	13.787	-59.977	-36.548	4.698
1800	11.869	61.965	53.652	14.964	-60.041	-35.167	4.270
1900	12.048	62.612	54.107	16.160	-60.098	-33.784	3.886
2000	12.214	63.234	54.548	17.373	-60.150	-32.398	3.540

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.895 + 2.882\times10^{-3}T + 0.240\times10^{5}T^{-2}$

$H°- H°_{298} = 6.895\times10^{-3}T + 1.441\times10^{-6}T^{2} - 0.240\times10^{2}T^{-1} - 2.103$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -56.816 - 3.176\times10^{-3}T + 0.771\times10^{-6}T^{2} - 30.100T^{-1}$

$\Delta Gf° = -56.816 + 3.176\times10^{-3}T\ln T - 0.771\times10^{-6}T^{2} - 15.050T^{-1} - 10.378\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (36). All other data from JANAF (51).

$D_2O(g)$

Dideutero-water (ideal gas)

[Formation: $D_2(g) + 0.5O_2(g) = D_2O(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.187	47.378	47.378	0	-59.561	-56.059	41.092
300	8.193	47.429	47.379	.015	-59.566	-56.038	40.823
400	8.517	49.828	47.703	.850	-59.784	-54.828	29.956
500	8.887	51.768	48.328	1.720	-59.979	-53.566	23.413
600	9.282	53.423	49.043	2.628	-60.154	-52.267	19.038
700	9.691	54.884	49.774	3.577	-60.306	-50.939	15.904
800	10.098	56.205	50.498	4.566	-60.439	-49.593	13.548
900	10.490	57.417	51.199	5.596	-60.552	-48.230	11.712
1000	10.857	58.542	51.878	6.664	-60.646	-46.856	10.240
1100	11.192	59.593	52.533	7.766	-60.727	-45.474	9.035
1200	11.494	60.580	53.163	8.901	-60.792	-44.083	8.028
1300	11.765	61.510	53.768	10.064	-60.847	-42.687	7.176
1400	12.007	62.391	54.353	11.253	-60.891	-41.290	6.446
1500	12.222	63.227	54.918	12.464	-60.928	-39.889	5.812
1600	12.413	64.022	55.462	13.696	-60.956	-38.485	5.257
1700	12.584	64.780	55.988	14.946	-60.979	-37.080	4.767
1800	12.737	65.504	56.497	16.213	-60.997	-35.673	4.331
1900	12.874	66.196	56.989	17.493	-61.013	-34.266	3.941
2000	12.998	66.860	57.466	18.787	-61.025	-32.859	3.591

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.413 + 3.256\times10^{-3}T - 0.175\times10^{5}T^{-2}$

$H°- H°_{298} = 7.413\times10^{-3}T + 1.628\times10^{-6}T^{2} + 0.175\times10^{2}T^{-1} - 2.414$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -58.976 - 2.466\times10^{-3}T + 0.748\times10^{-6}T^{2} + 25.000T^{-1}$

$\Delta Gf° = -58.976 + 2.466\times10^{-3}T\ln T - 0.748\times10^{-6}T^{2} + 12.500T^{-1} - 4.185\times10^{-3}T$

Source: Data from JANAF (53).

$H_2O_2(g)$

Hydrogen Peroxide (ideal gas)

[Formation: $H_2(g) + O_2(g) = H_2O_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.115	56.009	56.009	0	-32.580	-25.364	18.592
300	10.132	56.072	56.009	.019	-32.587	-25.319	18.445
400	11.080	59.116	56.419	1.079	-32.931	-22.843	12.480
500	11.961	61.686	57.222	2.232	-33.208	-20.288	8.868
600	12.702	63.934	58.156	3.467	-33.428	-17.681	6.440
700	13.317	65.940	59.127	4.769	-33.606	-15.042	4.696
800	13.838	67.753	60.094	6.127	-33.752	-12.381	3.382
900	14.292	69.410	61.039	7.534	-33.870	-9.702	2.356
1000	14.696	70.937	61.953	8.984	-33.965	-7.012	1.532
1100	15.060	72.355	62.835	10.472	-34.042	-4.312	.857
1200	15.390	73.680	63.685	11.994	-34.104	-1.607	.293
1300	15.689	74.923	64.501	13.548	-34.152	1.104	-.186
1400	15.959	76.096	65.287	15.132	-34.188	3.818	-.596
1500	16.202	77.206	66.047	16.739	-34.218	6.531	-.952

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 10.210 + 4.564\times10^{-3}T - 1.294\times10^{5}T^{-2}$

$H°- H°_{298} = 10.210\times10^{-3}T + 2.282\times10^{-6}T^{2} + 1.294\times10^{2}T^{-1} - 3.681$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf° = -32.002 - 3.476\times10^{-3}T + 1.360\times10^{-6}T^{2} + 100.700T^{-1}$

$\Delta Gf° = -32.002 + 3.476\times10^{-3}T\ln T - 1.360\times10^{-6}T^{2} + 50.350T^{-1} + 2.300\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from Chao (30).

He(g)

Helium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	4.968	30.125	30.125	0
300	4.968	30.156	30.126	.009
400	4.968	31.585	30.320	.506
500	4.968	32.693	30.687	1.003
600	4.968	33.599	31.099	1.500
700	4.968	34.365	31.514	1.996
800	4.968	35.028	31.912	2.493
900	4.968	35.614	32.292	2.990
1000	4.968	36.137	32.650	3.487
1100	4.968	36.610	32.988	3.984
1200	4.968	37.043	33.310	4.480
1300	4.968	37.440	33.612	4.977
1400	4.968	37.809	33.899	5.474
1500	4.968	38.151	34.170	5.971
1600	4.968	38.472	34.430	6.468
1700	4.968	38.773	34.677	6.964
1800	4.968	39.057	34.912	7.461
1900	4.968	39.326	35.138	7.958
2000	4.968	39.581	35.354	8.455
2100	4.968	39.823	35.560	8.952
2200	4.968	40.054	35.759	9.448
2300	4.968	40.275	35.951	9.945
2400	4.968	40.486	36.135	10.442
2500	4.968	40.689	36.313	10.939
2600	4.968	40.884	36.486	11.436
2700	4.968	41.071	36.652	11.932
2800	4.968	41.252	36.813	12.429
2900	4.968	41.426	36.969	12.926
3000	4.968	41.595	37.121	13.423

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $C_p^\circ = 4.968$

$H^\circ - H^\circ_{298} = 4.968 \times 10^{-3} T - 1.481$

Source: Data from JANAF (52).

Hf(c,l)

Hafnium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.150	10.410	10.410	0
300	6.150	10.450	10.413	.011
400	6.340	12.240	10.650	.636
500	6.520	13.680	11.124	1.278
600	6.700	14.880	11.648	1.939
700	6.880	15.930	12.190	2.618
800	7.060	16.860	12.715	3.316
900	7.250	17.700	13.221	4.031
1000	7.430	18.470	13.705	4.765
1100	7.610	19.190	14.175	5.517
1200	7.790	19.860	14.621	6.287
1300	7.980	20.490	15.047	7.076
1400	8.160	21.090	15.460	7.882
1500	8.340	21.660	15.855	8.707
1600	8.520	22.200	16.231	9.550
1700	8.700	22.720	16.595	10.412
1800	8.890	23.230	16.957	11.291
1900	9.070	23.710	17.295	12.189
2000	9.250	24.180	17.628	13.105
2013	9.270	24.240	17.670	13.225
2013*	7.887	25.040	17.670	14.835
2100	7.979	25.375	17.982	15.525
2200	8.147	25.750	18.327	16.331
2300	8.380	26.117	18.658	17.156
2400	8.679	26.480	18.976	18.009
2470	8.927	26.733	19.193	18.625
2470	8.000	29.033	19.193	24.305
2500	8.000	29.129	19.311	24.545
2600	8.000	29.443	19.695	25.345
2700	8.000	29.745	20.062	26.145
2800	8.000	30.036	20.413	26.945
2900	8.000	30.317	20.750	27.745
3000	8.000	30.588	21.073	28.545

*Entropies of transition and fusion, and data for Hf(l) estimated.

Phase changes: 2013 K, α - β transition point of Hf; ΔH° = 1.610 kcal/mol.
2470 K, melting point of Hf; ΔH° = 5.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2013 K: $Cp^\circ = 5.609 + 1.820\times10^{-3}T$

$H^\circ - H^\circ_{298} = 5.609\times10^{-3}T + 0.910\times10^{-6}T^2 - 1.753$

2013-2470 K: $Cp^\circ = 3.429 + 2.170\times10^{-3}T$

$H^\circ - H^\circ_{298} = 3.429\times10^{-3}T + 1.085\times10^{-6}T^2 + 3.536$

2470-3000 K: $Cp^\circ = 8.000$

$H^\circ - H^\circ_{298} = 8.000\times10^{-3}T + 4.545$

Sources: Data 298 to 2013 K, including estimated entropy of transition, from Hultgren (99). Data from 2013 to 2470 K based on Cezairliyan (24). Temperature of fusion from Cezairliyan (25). Entropy of fusion and heat capacity of Hf(l) are those estimated by Hultgren.

Hf(g)

Hafnium (ideal monatomic gas)

[Formation: Hf(c,1) = Hf(g)]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.972	44.643	44.643	0	148.000	137.793	-101.004
300	4.972	44.674	44.644	.009	147.998	137.731	-100.336
400	5.010	46.108	44.838	.508	147.872	134.325	-73.391
500	5.114	47.236	45.210	1.013	147.735	130.957	-57.241
600	5.285	48.182	45.627	1.533	147.594	127.613	-46.482
700	5.500	49.013	46.053	2.072	147.454	124.296	-38.806
800	5.734	49.762	46.470	2.634	147.318	120.996	-33.054
900	5.970	50.451	46.874	3.219	147.188	117.712	-28.584
1000	6.196	51.092	47.265	3.827	147.062	114.440	-25.011
1100	6.407	51.693	47.641	4.457	146.940	111.187	-22.090
1200	6.596	52.259	48.002	5.108	146.821	107.942	-19.659
1300	6.763	52.793	48.350	5.776	146.700	104.706	-17.602
1400	6.906	53.300	48.686	6.460	146.578	101.484	-15.842
1500	7.026	53.781	49.010	7.156	146.449	98.268	-14.317
1600	7.123	54.237	49.322	7.864	146.314	95.055	-12.984
1700	7.200	54.672	49.625	8.580	146.168	91.850	-11.808
1800	7.260	55.085	49.916	9.304	146.013	88.674	-10.766
1900	7.305	55.479	50.199	10.032	145.843	85.482	-9.833
2000	7.338	55.854	50.472	10.764	145.659	82.311	-8.994
2013	7.341	55.902	50.507	10.859	145.634	81.900	-8.892
2013	7.341	55.902	50.507	10.859	144.024	81.900	-8.892
2100	7.362	56.213	50.737	11.499	143.974	79.214	-8.244
2200	7.379	56.556	50.994	12.236	143.905	76.132	-7.563
2300	7.392	56.884	51.243	12.975	143.819	73.055	-6.942
2400	7.403	57.199	51.484	13.715	143.706	69.980	-6.373
2470	7.411	57.412	51.649	14.233	143.608	67.833	-6.002
2470	7.411	57.412	51.649	14.233	137.928	67.833	-6.002
2500	7.415	57.501	51.719	14.455	137.910	66.980	-5.855

Phase changes: 2013 K, α - β transition point of Hf; $\Delta H° = 1.610$ kcal/mol.
2470 K, melting point of Hf; $\Delta H° = 5.680$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 4.462 + 1.550\times10^{-3}T + 0.043\times10^{5}T^{-2}$

$H°- H°_{298} = 4.462\times10^{-3}T + 0.775\times10^{-6}T^{2} - 0.043\times10^{2}T^{-1} - 1.385$

Formation equations (kcal/mol):

298.15-2013 K: $\Delta Hf° = 148.368 - 1.147\times10^{-3}T - 0.135\times10^{-6}T^{2} - 4.300T^{-1}$

$\Delta Gf° = 148.368 + 1.147\times10^{-3}T\ln T + 0.135\times10^{-6}T^{2} - 2.150T^{-1} - 42.020\times10^{-3}T$

2013-2470 K: $\Delta Hf° = 143.079 + 1.033\times10^{-3}T - 0.310\times10^{-6}T^{2} - 4.300T^{-1}$

$\Delta Gf° = 143.079 - 1.033\times10^{-3}T\ln T + 0.310\times10^{-6}T^{2} - 2.150T^{-1} - 23.160\times10^{-3}T$

2470-2500 K: $\Delta Hf° = 142.070 - 3.538\times10^{-3}T + 0.775\times10^{-6}T^{2} - 4.300T^{-1}$

$\Delta Gf° = 142.070 + 3.538\times10^{-3}T\ln T - 0.775\times10^{-6}T^{2} - 2.150T^{-1} - 55.781\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (238). All other from Hilsenrath (94).

HfO_2(c)

Hafnium Dioxide

[Formation: $Hf(c) + O_2(g) = HfO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.400	14.180	14.180	0	-267.120	-253.633	185.916
300	14.441	14.269	14.180	.027	-267.117	-253.548	184.707
400	15.996	18.651	14.766	1.554	-266.925	-249.053	136.075
500	16.963	22.332	15.922	3.205	-266.647	-244.613	106.919
600	17.640	25.488	17.260	4.937	-266.331	-240.238	87.505
700	18.153	28.247	18.636	6.728	-265.997	-235.912	73.654
800	18.560	30.698	19.993	8.564	-265.657	-231.639	63.280
900	18.894	32.904	21.307	10.437	-265.313	-227.409	55.222
1000	19.174	34.910	22.569	12.341	-264.970	-223.220	48.784
1100	19.416	36.749	23.775	14.271	-264.631	-219.057	43.522
1200	19.634	38.448	24.929	16.223	-264.297	-214.929	39.143
1300	19.836	40.028	26.030	18.197	-263.968	-210.830	35.443
1400	20.034	41.505	27.084	20.190	-263.645	-206.752	32.275
1500	20.236	42.894	28.091	22.204	-263.326	-202.697	29.533
1600	20.453	44.207	29.058	24.238	-263.012	-198.673	27.137
1700	20.691	45.454	29.986	26.295	-262.699	-194.665	25.026
1800	20.961	46.644	30.879	28.377	-262.384	-190.658	23.149

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 17.014 + 2.340\times10^{-3}T - 2.944\times10^{5}T^{-2}$

$H°- H°_{298} = 17.014\times10^{-3}T + 1.170\times10^{-6}T^{2} + 2.944\times10^{2}T^{-1} - 6.164$

Formation equations (kcal/mol):

298.15-1800 K: $\Delta Hf° = -269.179 + 4.175\times10^{-3}T - 0.243\times10^{-6}T^{2} + 249.200T^{-1}$

$\Delta Gf° = -269.179 - 4.175\times10^{-3}T\ln T + 0.243\times10^{-6}T^{2} + 124.600T^{-1} + 74.454\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kornilov (138). Low-temperature heat capacities and entropy at 298 K from Todd (222). High-temperature data based on Orr (170).

Hg(l,g)

Mercury

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ-H^\circ_{298})/T$	kcal/mol
298.15	6.687	18.140	18.140	0
300	6.684	18.181	18.141	.012
400	6.552	20.084	18.401	.673
500	6.495	21.539	18.889	1.325
600	6.486	22.721	19.431	1.974
629.81	6.497	23.038	19.597	2.167
629.81	4.968	45.507	19.597	16.318
700	4.968	46.032	22.223	16.666
800	4.968	46.695	25.241	17.163
900	4.968	47.281	27.659	17.660
1000	4.968	47.804	29.647	18.157
1100	4.968	48.277	31.319	18.654
1200	4.968	48.710	32.751	19.151
1300	4.968	49.107	33.994	19.647
1400	4.968	49.476	35.087	20.144
1500	4.968	49.818	36.057	20.641
1600	4.968	50.139	36.928	21.138
1700	4.968	50.440	37.714	21.635
1800	4.968	50.724	38.429	22.131
1900	4.968	50.993	39.084	22.628
2000	4.968	51.248	39.686	23.125

Phase changes: 234.29 K, melting point of Hg; ΔH° = 0.549 kcal/mol.
629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-629.81 K: $Cp^\circ = 6.273 + 0.202\times10^{-3}T + 0.314\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.273\times10^{-3}T + 0.101\times10^{-6}T^2 - 0.314\times10^{2}T^{-1} - 1.774$

629.81-2000 K: $Cp^\circ = 4.968$

$H^\circ - H^\circ_{298} = 4.968\times10^{-3}T + 13.189$

Sources: Entropy of Hg(l) at 298 K and entropy and enthalpy of formation of Hg(g) at 298 K from CODATA (36). All other data from JANAF (51).

Hg(g)

Mercury (ideal monatomic gas)

[Formation: Hg(l,g) = Hg(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	4.968	41.792	41.792	0	14.670	7.618	-5.584
300	4.968	41.822	41.792	.009	14.667	7.575	-5.518
400	4.968	43.252	41.987	.506	14.503	5.236	-2.861
500	4.968	44.360	42.354	1.003	14.348	2.938	-1.284
600	4.968	45.266	42.766	1.500	14.196	.669	-.244
629.81	4.968	45.507	42.890	1.648	14.151	0	0
629.81	4.968	45.507	42.890	1.648	0	0	0
700	4.968	46.032	43.181	1.996	0	0	0
800	4.968	46.695	43.579	2.493	0	0	0
900	4.968	47.281	43.959	2.990	0	0	0
1000	4.968	47.804	44.317	3.487	0	0	0
1100	4.968	48.277	44.655	3.984	0	0	0
1200	4.968	48.710	44.976	4.481	0	0	0
1300	4.968	49.107	45.279	4.977	0	0	0
1400	4.968	49.476	45.566	5.474	0	0	0
1500	4.968	49.818	45.837	5.971	0	0	0
1600	4.968	50.139	46.097	6.468	0	0	0
1700	4.968	50.440	46.343	6.965	0	0	0
1800	4.968	50.724	46.579	7.461	0	0	0
1900	4.968	50.993	46.805	7.958	0	0	0
2000	4.968	51.248	47.021	8.455	0	0	0

Phase change: 629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 4.968$

$H^\circ - H^\circ_{298} = 4.968 \times 10^{-3} T - 1.481$

Formation equations (kcal/mol):

298.15-629.81 K: $\Delta Hf^\circ = 14.963 - 1.305 \times 10^{-3} T - 0.101 \times 10^{-6} T^2 + 31.400 T^{-1}$

$\Delta Gf^\circ = 14.963 + 1.305 \times 10^{-3} T \ln T + 0.101 \times 10^{-6} T^2 + 15.700 T^{-1} - 32.276 \times 10^{-3} T$

629.81-2000 K: $\Delta Hf^\circ = 0$

$\Delta Gf^\circ = 0$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (36). All other data from JANAF (51).

HgO(c)

Mercury Oxide

[Formation: $Hg(l,g) + 0.5O_2(g) = HgO(s)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.531	16.795	16.795	0	-21.700	-13.994	10.257
300*	10.551	16.860	16.793	.020	-21.698	-13.945	10.159
400	11.550	20.037	17.222	1.126	-21.609	-11.372	6.213
500	12.340	22.703	18.057	2.323	-21.429	-8.831	3.860
600	12.935	25.008	19.030	3.587	-21.192	-6.335	2.307
629.81	13.074	25.639	19.328	3.975	-21.112	-5.596	1.942
629.81	13.074	25.639	19.328	3.975	-35.263	-5.596	1.942
700	13.400	27.038	20.031	4.905	-34.955	-2.305	.720
749	13.580	27.951	20.520	5.566	-34.731	-.028	.008

*Data above 298 K estimated.

Phase change: 629.81 K, boiling point of Hg; $\Delta H° = 14.151$ kcal/mol.
749 K, decomposition point of HgO.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-749 K: $Cp° = 10.341 + 4.764\times10^{-3}T - 1.094\times10^{5}T^{-2}$

$H°- H°_{298} = 10.341\times10^{-3}T + 2.382\times10^{-6}T^{2} + 1.094\times10^{2}T^{-1} - 3.662$

Formation equations (kcal/mol):

298.15-629.81 K: $\Delta Hf° = -22.412 + 0.453\times10^{-3}T + 2.030\times10^{-6}T^{2} + 118.200T^{-1}$

$\Delta Gf° = -22.412 - 0.453\times10^{-3}T\ln T - 2.030\times10^{-6}T^{2} + 59.100T^{-1} + 30.757\times10^{-3}T$

629.81-749 K: $\Delta Hf° = -37.375 + 1.758\times10^{-3}T + 2.131\times10^{-6}T^{2} + 86.800T^{-1}$

$\Delta Gf° = -37.375 - 1.758\times10^{-3}T\ln T - 2.131\times10^{-6}T^{2} + 43.400T^{-1} + 63.029\times10^{-3}T$

Source: Data from JANAF (51) who estimated data above 298 K.

HgO(g)

Mercury Oxide (ideal gas)

[Formation: $Hg(l,g) + 0.5O_2(g) = HgO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.859	57.134	57.134	0	10.000	5.679	-4.163
300	7.868	57.183	57.134	.015	9.997	5.653	-4.118
400	8.236	59.500	57.447	.821	9.786	4.238	-2.316
500	8.469	61.365	58.051	1.657	9.605	2.872	-1.255
600	8.620	62.923	58.736	2.512	9.434	1.541	-.561
629.81	8.651	63.342	58.944	2.769	9.383	1.152	-.400
629.81	8.651	63.342	58.944	2.769	-4.768	1.152	-.400
700	8.724	64.261	59.432	3.380	-4.780	1.814	-.566
800	8.798	65.431	60.111	4.256	-4.799	2.756	-.753
900	8.854	66.470	60.760	5.139	-4.820	3.703	-.899
1000	8.898	67.405	61.379	6.026	-4.844	4.650	-1.016
1100	8.934	68.255	61.966	6.918	-4.868	5.600	-1.113
1200	8.964	69.034	62.523	7.813	-4.894	6.554	-1.194
1300	8.990	69.752	63.051	8.711	-4.920	7.509	-1.262
1400	9.012	70.419	63.554	9.611	-4.949	8.467	-1.322
1500	9.033	71.042	64.033	10.513	-4.979	9.424	-1.373
1600	9.052	71.625	64.489	11.417	-5.011	10.387	-1.419
1700	9.069	72.175	64.926	12.323	-5.043	11.348	-1.459
1800	9.086	72.694	65.343	13.231	-5.075	12.315	-1.495
1900	9.101	73.185	65.743	14.140	-5.110	13.283	-1.528
2000	9.116	73.652	66.127	15.051	-5.146	14.253	-1.557

*All data estimated.

Phase change: 629.81 K, boiling point of Hg; $\Delta H° = 14.151$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.671 + 0.274\times10^{-3}T - 0.794\times10^{5}T^{-2}$

$H°- H°_{298} = 8.671\times10^{-3}T + 0.137\times10^{-6}T^{2} + 0.794\times10^{2}T^{-1} - 2.864$

Formation equations (kcal/mol):

298.15-629.81 K: $\Delta Hf° = 10.086 - 1.217\times10^{-3}T - 0.215\times10^{-6}T^{2} + 88.200T^{-1}$

$\Delta Gf° = 10.086 + 1.217\times10^{-3}T\ln T + 0.215\times10^{-6}T^{2} + 44.100T^{-1} - 22.275\times10^{-3}T$

629.81-2000 K: $\Delta Hf° = -4.877 + 0.088\times10^{-3}T - 0.114\times10^{-6}T^{2} + 56.800T^{-1}$

$\Delta Gf° = -4.877 - 0.088\times10^{-3}T\ln T + 0.114\times10^{-6}T^{2} + 28.400T^{-1} + 9.998\times10^{-3}T$

Source: Data are those estimated by JANAF (51).

Ho(c,l)

Holmium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.490	17.930	17.930	0
300	6.490	17.970	17.930	.012
400	6.650	19.860	18.185	.670
500	6.740	21.360	18.680	1.340
600	6.760	22.590	19.230	2.016
700	6.800	23.630	19.786	2.691
800	6.950	24.550	20.327	3.378
900	7.270	25.390	20.847	4.089
1000	7.610	26.170	21.338	4.832
1100	8.070	26.910	21.805	5.615
1200	8.580	27.640	22.267	6.447
1300	9.200	28.350	22.707	7.336
1400	9.890	29.060	23.138	8.291
1500	10.690	29.770	23.557	9.319
1600	11.540	30.480	23.962	10.429
1700	12.450	31.210	24.370	11.628
1701	12.460	31.210	24.367	11.641
1701*	6.700	31.870	24.367	12.762
1743	6.700	32.040	24.557	13.043
1743	10.500	33.710	24.557	15.954
1800	10.500	34.050	24.854	16.553
1900	10.500	34.610	25.345	17.603
2000	10.500	35.150	25.824	18.653

*Data for Ho(β) and Ho(l) estimated.

Phase changes: 1701 K, α - β transition point of Ho; ΔH° = 1.121 kcal/mol.
1743 K, melting point of Ho; ΔH° = 2.911 kcal/mol.
2968 K, boiling point of Ho; ΔH° = 57.6 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1701 K: $Cp^\circ = 3.341 + 4.650\times10^{-3}T + 1.567\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 3.341\times10^{-3}T + 2.325\times10^{-6}T^2 - 1.567\times10^{2}T^{-1} - 0.677$

1701-1743 K: $Cp^\circ = 6.700$

$H^\circ - H^\circ_{298} = 6.700\times10^{-3}T + 1.365$

1743-2000 K: $Cp^\circ = 10.500$

$H^\circ - H^\circ_{298} = 10.500\times10^{-3}T - 2.348$

Source: Data from Hultgren (99) who estimated data for Ho(β) and Ho(l).

Ho(g)

Holmium (ideal monatomic gas)

[Formation: Ho(c,1) = Ho(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^{\circ}_{298})/T$	$H°- H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	4.968	46.718	46.718	0	71.900	63.317	-46.412
300	4.968	46.749	46.719	.009	71.897	63.263	-46.087
400	4.968	48.178	46.913	.506	71.736	60.409	-33.005
500	4.968	49.287	47.281	1.003	71.563	57.600	-25.176
600	4.969	50.192	47.692	1.500	71.384	54.823	-19.969
700	4.971	50.958	48.105	1.997	71.206	52.076	-16.259
800	4.978	51.623	48.506	2.494	71.016	49.358	-13.484
900	4.991	52.210	48.886	2.992	70.803	46.665	-11.332
1000	5.012	52.736	49.244	3.492	70.560	43.994	-9.615
1100	5.042	53.215	49.583	3.995	70.280	41.345	-8.214
1200	5.083	53.656	49.905	4.501	69.954	38.735	-7.054
1300	5.132	54.065	50.210	5.012	69.576	36.147	-6.077
1400	5.188	54.447	50.498	5.528	69.137	33.595	-5.244
1500	5.251	54.807	50.774	6.050	68.631	31.076	-4.528
1600	5.320	55.148	51.037	6.578	68.049	28.580	-3.904
1700	5.392	55.473	51.288	7.114	67.386	26.139	-3.360
1701	5.393	55.476	51.291	7.119	67.378	26.103	-3.354
1701	5.393	55.476	51.291	7.119	66.257	26.103	-3.354
1743	5.424	55.608	51.393	7.347	66.204	25.124	-3.150
1743	5.424	55.608	51.393	7.347	63.293	25.124	-3.150
1800	5.466	55.783	51.529	7.657	63.004	23.885	-2.900
1900	5.541	56.080	51.761	8.207	62.504	21.711	-2.497
2000	5.616	56.367	51.985	8.765	62.012	19.578	-2.139

Phase changes: 1701 K, α - β transition point of Ho; $\Delta H°$ = 1.121 kcal/mol.
1743 K, melting point of Ho; $\Delta H°$ = 2.911 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.705 + 0.358\times10^{-3}T + 0.139\times10^{5}T^{-2}$

$H°- H^{\circ}_{298} = 4.705\times10^{-3}T + 0.179\times10^{-6}T^{2} - 0.139\times10^{2}T^{-1} - 1.372$

Formation equations (kcal/mol):

298.15-1701 K: $\Delta Hf° = 71.205 + 1.364\times10^{-3}T - 2.146\times10^{-6}T^{2} + 142.800T^{-1}$

$\Delta Gf° = 71.205 - 1.364\times10^{-3}T\ln T + 2.146\times10^{-6}T^{2} + 71.400T^{-1} - 20.129\times10^{-3}T$

1701-1743 K: $\Delta Hf° = 69.163 - 1.995\times10^{-3}T + 0.179\times10^{-6}T^{2} - 13.900T^{-1}$

$\Delta Gf° = 69.163 + 1.995\times10^{-3}T\ln T - 0.179\times10^{-6}T^{2} - 6.950T^{-1} - 39.934\times10^{-3}T$

1743-2000 K: $\Delta Hf° = 72.875 - 5.795\times10^{-3}T + 0.179\times10^{-6}T^{2} - 13.900T^{-1}$

$\Delta Gf° = 72.875 + 5.795\times10^{-3}T\ln T - 0.179\times10^{-6}T^{2} - 6.950T^{-1} - 70.425\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). All other data from Feber (58).

$Ho_2O_3(c)$

Diholmium Trioxide, Holmium Sesquioxide

[Formation: $2Ho(c,l) + 1.5O_2(g) = Ho_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	27.480	37.800	37.800	0	-449.550	-428.212	313.884
300	27.522	37.970	37.800	.051	-449.542	-428.079	311.852
400	29.082	46.133	38.903	2.892	-449.082	-420.994	230.017
500	29.864	52.715	41.029	5.843	-448.568	-414.025	180.968
600	30.349	58.206	43.448	8.855	-448.040	-407.169	148.309
700	30.695	62.911	45.900	11.908	-447.504	-400.399	125.009
800	30.968	67.028	48.288	14.992	-446.991	-393.702	107.553
900	31.199	70.690	50.578	18.101	-446.525	-387.064	93.991
1000	31.404	73.987	52.756	21.231	-446.122	-380.484	83.154
1100	31.591	76.989	54.824	24.381	-445.796	-373.949	74.296
1200	31.765	79.746	56.789	27.549	-445.564	-367.413	66.914
1300	31.930	82.295	58.653	30.734	-445.441	-360.910	60.674
1400	32.087	84.667	60.428	33.934	-445.448	-354.402	55.324
1500	32.236	86.886	62.119	37.151	-445.591	-347.891	50.687
1600	32.378	88.971	63.733	40.381	-445.897	-341.389	46.631
1700	32.513	90.938	65.276	43.626	-446.373	-334.831	43.045
1701	32.514	90.957	65.291	43.659	-446.380	-334.790	43.014
1701	32.514	90.957	65.291	43.659	-448.622	-334.790	43.014
1743	32.568	91.751	65.919	45.025	-448.376	-331.957	41.623
1743	32.568	91.751	65.919	45.025	-454.198	-331.957	41.623
1800	32.641	92.800	66.753	46.884	-454.297	-327.950	39.818
1900	32.761	94.568	68.171	50.154	-454.468	-320.956	36.918
2000	32.874	96.251	69.533	53.436	-454.634	-313.918	34.303

Phase changes: 1701 K, α - β transition point of Ho; $\Delta H° = 1.121$ kcal/mol.
1743 K, melting point of Ho; $\Delta H° = 2.911$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 30.364 + 1.332\times10^{-3}T - 2.917\times10^{5}T^{-2}$

$H°- H°_{298} = 30.364\times10^{-3}T + 0.666\times10^{-6}T^{2} + 2.917\times10^{2}T^{-1} - 10.091$

Formation equations (kcal/mol):

298.15-1701 K: $\Delta Hf° = -454.758 + 12.837\times10^{-3}T - 4.739\times10^{-6}T^{2} + 537.300T^{-1}$

$\Delta Gf° = -454.758 - 12.837\times10^{-3}T\ln T + 4.739\times10^{-6}T^{2} + 268.650T^{-1} + 157.741\times10^{-3}T$

1701-1743 K: $\Delta Hf° = -458.843 + 6.119\times10^{-3}T - 0.088\times10^{-6}T^{2} + 223.900T^{-1}$

$\Delta Gf° = -458.843 - 6.119\times10^{-3}T\ln T + 0.088\times10^{-6}T^{2} + 111.950T^{-1} + 118.131\times10^{-3}T$

1743-2000 K: $\Delta Hf° = -451.418 - 1.481\times10^{-3}T - 0.088\times10^{-6}T^{2} + 223.900T^{-1}$

$\Delta Gf° = -451.418 + 1.481\times10^{-3}T\ln T + 0.088\times10^{-6}T^{2} + 111.950T^{-1} + 57.150\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). Low-temperature heat capacities and entropy at 298 K from Westrum (248). High-temperature data based on Tsagareishvili (226) and Pankratz (178).

I_2(c,l,g)

Iodine

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	13.011	27.758	27.758	0
300	13.026	27.839	27.759	.024
386.8	15.188	31.365	28.180	1.232
386.8	19.281	40.954	28.180	4.941
400	19.281	41.602	28.612	5.196
458.4	19.281	44.232	30.443	6.321
458.4	8.930	66.093	30.443	16.342
500	8.948	66.873	33.445	16.714
600	8.980	68.507	39.155	17.611
700	9.005	69.893	43.450	18.510
800	9.025	71.097	46.833	19.411
900	9.044	72.161	49.589	20.315
1000	9.061	73.115	51.895	21.220
1100	9.077	73.979	53.864	22.127
1200	9.092	74.770	55.573	23.036
1300	9.107	75.498	57.079	23.945
1400	9.122	76.174	58.419	24.857
1500	9.137	76.803	59.623	25.770
1600	9.151	77.394	60.716	26.684
1700	9.165	77.949	61.714	27.600
1800	9.179	78.473	62.630	28.517
1900	9.193	78.970	63.477	29.436
2000	9.207	79.442	64.264	30.356
2100	9.220	79.891	64.997	31.277
2200	9.234	80.320	65.684	32.200
2300	9.248	80.731	66.329	33.124
2400	9.261	81.125	66.938	34.050
2500	9.275	81.503	67.513	34.976
2600	9.289	81.867	68.057	35.905
2700	9.302	82.218	68.576	36.834
2800	9.316	82.557	69.069	37.765
2900	9.329	82.884	69.540	38.697
3000	9.343	83.200	69.990	39.631

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2: ΔH° = 10.021 Kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-386.8 K: $Cp^\circ = 12.877 + 2.984\times10^{-3}T$

$H^\circ - H^\circ_{298} = 12.877\times10^{-3}T + 1.492\times10^{-6}T^2 - 3.972$

386.8-458.4 K: $Cp^\circ = 19.281$

$H^\circ - H^\circ_{298} = 19.281\times10^{-3}T - 2.517$

458.4-3000 K: $Cp^\circ = 8.941 + 0.136\times10^{-3}T - 0.153\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.941\times10^{-3}T + 0.068\times10^{-6}T^2 + 0.153\times10^{2}T^{-1} + 12.196$

Sources: Entropy of I_2(s) at 298 K and enthalpy of formation of I_2(g) at 298 K from CODATA (36). All other data from JANAF (51).

I(g)

Iodine (ideal monatomic gas)

[Formation: $0.5I_2(c,l,g) = I(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	43.182	43.182	0	25.517	16.780	-12.300
300	4.968	43.213	43.183	.009	25.514	16.726	-12.185
386.8	4.968	44.475	43.337	.440	25.341	14.204	-8.026
386.8	4.968	44.475	43.337	.440	23.487	14.204	-8.026
400	4.968	44.642	43.377	.506	23.425	13.889	-7.588
458.4	4.968	45.319	43.582	.796	23.153	12.516	-5.967
458.4	4.968	45.319	43.582	.796	18.142	12.516	-5.967
500	4.968	45.751	43.745	1.003	18.163	12.006	-5.248
600	4.968	46.656	44.156	1.500	18.212	10.770	-3.923
700	4.968	47.422	44.571	1.996	18.258	9.525	-2.974
800	4.968	48.086	44.970	2.493	18.305	8.275	-2.260
900	4.969	48.671	45.349	2.990	18.350	7.018	-1.704
1000	4.970	49.194	45.707	3.487	18.394	5.757	-1.258
1100	4.973	49.668	46.046	3.984	18.438	4.491	-.892
1200	4.977	50.101	46.366	4.482	18.481	3.222	-.587
1300	4.983	50.500	46.669	4.980	18.524	1.948	-.328
1400	4.992	50.869	46.956	5.478	18.567	.672	-.105
1500	5.004	51.214	47.229	5.978	18.610	-.609	.089
1600	5.018	51.537	47.488	6.479	18.654	-1.890	.258
1700	5.034	51.842	47.735	6.982	18.699	-3.176	.408
1800	5.052	52.130	47.971	7.486	18.745	-4.464	.542
1900	5.072	52.404	48.198	7.992	18.791	-5.755	.662
2000	5.093	52.665	48.415	8.500	18.839	-7.049	.770
2100	5.114	52.914	48.623	9.011	18.889	-8.344	.868
2200	5.137	53.152	48.823	9.523	18.940	-9.642	.958
2300	5.160	53.381	49.017	10.038	18.993	-10.943	1.040
2400	5.182	53.601	49.203	10.555	19.047	-12.245	1.115
2500	5.204	53.813	49.383	11.074	19.103	-13.551	1.185
2600	5.226	54.017	49.557	11.596	19.160	-14.857	1.249
2700	5.247	54.215	49.726	12.120	19.220	-16.166	1.309
2800	5.267	54.406	49.890	12.645	19.280	-17.477	1.364
2900	5.286	54.591	50.049	13.173	19.342	-18.791	1.416
3000	5.304	54.771	50.204	13.702	19.404	-20.110	1.465

Phase changes: 386.8 K, melting point of I_2; $\Delta H° = 3.709$ kcal/mol.
458.4 K, boiling point of I_2; $\Delta H° = 10.021$ kcal/mol of I_2.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 4.880 + 0.104\times10^{-3}T + 0.050\times10^{5}T^{-2}$

$H°-H°_{298} = 4.880\times10^{-3}T + 0.052\times10^{-6}T^2 - 0.050\times10^{2}T^{-1} - 1.443$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = 26.060 - 1.558\times10^{-3}T - 0.694\times10^{-6}T^2 - 5.000T^{-1}$

$\Delta Gf° = 26.060 + 1.558\times10^{-3}T\ln T + 0.694\times10^{-6}T^2 - 2.500T^{-1} - 40.183\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = 25.333 - 4.760\times10^{-3}T + 0.052\times10^{-6}T^2 - 5.000T^{-1}$

$\Delta Gf° = 25.333 + 4.760\times10^{-3}T\ln T - 0.052\times10^{-6}T^2 - 2.500T^{-1} - 57.091\times10^{-3}T$

458.4-3000 K: $\Delta Hf° = 17.976 + 0.409\times10^{-3}T + 0.018\times10^{-6}T^2 - 12.650T^{-1}$

$\Delta Gf° = 17.976 - 0.409\times10^{-3}T\ln T - 0.018\times10^{-6}T^2 - 6.325T^{-1} - 9.359\times10^{-3}T$

Source: Data from Chase (33).

$I_2(g)$

Iodine (ideal diatomic gas)

[Formation: $I_2(c,l,g) = I_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.814	62.277	62.277	0	14.919	4.627	-3.392
300	8.817	62.332	62.279	.016	14.911	4.563	-3.324
386.8	8.890	64.582	62.552	.786	14.473	1.624	-.918
386.8	8.890	64.582	62.552	.786	10.764	1.624	-.918
400	8.901	64.881	62.623	.903	10.626	1.314	-.718
458.4	8.928	66.097	62.992	1.423	10.021	0	0
458.4	8.928	66.097	62.992	1.423	0	0	0
500	8.948	66.873	63.283	1.795	0	0	0
600	8.980	68.507	64.020	2.692	0	0	0
700	9.005	69.893	64.763	3.591	0	0	0
800	9.025	71.097	65.482	4.492	0	0	0
900	9.044	72.161	66.165	5.396	0	0	0
1000	9.061	73.115	66.814	6.301	0	0	0
1100	9.077	73.979	67.426	7.208	0	0	0
1200	9.092	74.770	68.006	8.117	0	0	0
1300	9.107	75.498	68.554	9.027	0	0	0
1400	9.122	76.174	69.075	9.938	0	0	0
1500	9.137	76.803	69.569	10.851	0	0	0
1600	9.151	77.394	70.041	11.765	0	0	0
1700	9.165	77.949	70.490	12.681	0	0	0
1800	9.179	78.473	70.919	13.598	0	0	0
1900	9.193	78.970	71.329	14.517	0	0	0
2000	9.207	79.442	71.724	15.437	0	0	0
2100	9.220	79.891	72.101	16.358	0	0	0
2200	9.234	80.320	72.465	17.281	0	0	0
2300	9.248	80.731	72.816	18.205	0	0	0
2400	9.261	81.125	73.154	19.131	0	0	0
2500	9.275	81.503	73.480	20.057	0	0	0
2600	9.289	81.867	73.795	20.986	0	0	0
2700	9.302	82.218	74.101	21.915	0	0	0
2800	9.316	82.557	74.398	22.846	0	0	0
2900	9.329	82.884	74.685	23.778	0	0	0
3000	9.343	83.200	74.963	24.712	0	0	0

Phase changes: 386.8 K, melting point of I_2; $\Delta H° = 3.709$ kcal/mol.
458.4 K, boiling point of I_2; $\Delta H° = 10.021$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 8.939 + 0.136\times10^{-3}T - 0.147\times10^{5}T^{-2}$

$H°- H°_{298} = 8.939\times10^{-3}T + 0.068\times10^{-6}T^2 + 0.147\times10^{2}T^{-1} - 2.721$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = 16.170 - 3.938\times10^{-3}T - 1.424\times10^{-6}T^2 + 14.700T^{-1}$

$\Delta Gf° = 16.170 + 3.938\times10^{-3}T\ln T + 1.424\times10^{-6}T^2 + 7.350T^{-1} - 61.661\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = 14.715 - 10.342\times10^{-3}T + 0.068\times10^{-6}T^2 + 14.700T^{-1}$

$\Delta Gf° = 14.715 + 10.342\times10^{-3}T\ln T - 0.068\times10^{-6}T^2 + 7.350T^{-1} - 95.476\times10^{-3}T$

458.4-3000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (36). All other data from JANAF (51).

In(c,1)

Indium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.389	13.820	13.820	0
300	6.391	13.860	13.820	.012
400	6.925	15.763	14.073	.676
429.78	7.250	16.270	14.209	.886
429.78	7.050	18.085	14.209	1.666
500	7.030	19.150	14.830	2.160
600	7.010	20.430	15.660	2.862
700	6.990	21.509	16.420	3.562
800	6.970	22.441	17.116	4.260
900*	6.950	23.261	17.754	4.956
1000	6.950	23.993	18.342	5.651
1100	6.950	24.656	18.887	6.346
1200	6.950	25.260	19.392	7.041
1300	6.950	25.816	19.865	7.736
1400	6.950	26.332	20.310	8.431
1500	6.950	26.812	20.728	9.126
1600	6.950	27.260	21.122	9.821
1700	6.950	27.682	21.496	10.516
1800	6.950	28.078	21.850	11.211
1900	6.950	28.454	22.188	11.906
2000	6.950	28.810	22.510	12.601

*Data above 800 K extrapolated.

Phase changes: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
2346 K, boiling point of In; ΔH° = 55.3 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-429.78 K: $Cp^\circ = 2.620 + 9.524\times10^{-3}T + 0.827\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 2.620\times10^{-3}T + 4.762\times10^{-6}T^{2} - 0.827\times10^{2}T^{-1} - 0.927$

429.78-2000 K: $Cp^\circ = 6.967 - 0.020\times10^{-3}T + 0.170\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.967\times10^{-3}T - 0.010\times10^{-6}T^{2} - 0.170\times10^{2}T^{-1} - 1.287$

Source: Data from Hultgren (99) who extrapolated above 800 K by assuming constant heat capacity.

In(g)

Indium (ideal monatomic gas)

[Formation: In(c,l) = In(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^{\circ}_{298})/T$	$H°- H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	4.979	41.508	41.508	0	58.150	49.895	-36.573
300	4.979	41.538	41.508	.010	58.148	49.845	-36.311
400	5.056	42.979	41.704	.510	57.984	47.098	-25.733
429.78	5.112	43.344	41.805	.661	57.925	46.290	-23.539
429.78	5.112	43.344	41.805	.661	57.145	46.290	-23.539
500	5.243	44.125	42.077	1.024	57.014	44.526	-19.462
600	5.512	45.104	42.501	1.562	56.850	42.046	-15.315
700	5.803	45.976	42.937	2.127	56.715	39.588	-12.360
800	6.062	46.768	43.367	2.721	56.611	37.149	-10.149
900	6.260	47.494	43.785	3.338	56.532	34.722	-8.432
1000	6.391	48.161	44.190	3.971	56.470	32.302	-7.060
1100	6.462	48.774	44.579	4.614	56.418	29.888	-5.938
1200	6.482	49.337	44.953	5.261	56.370	27.478	-5.004
1300	6.465	49.856	45.311	5.909	56.323	25.071	-4.215
1400	6.422	50.334	45.653	6.554	56.273	22.670	-3.539
1500	6.363	50.775	45.980	7.193	56.217	20.273	-2.954
1600	6.295	51.183	46.292	7.826	56.155	17.878	-2.442
1700	6.221	51.563	46.591	8.452	56.086	15.488	-1.991
1800	6.147	51.916	46.877	9.070	56.009	13.101	-1.591
1900	6.074	52.246	47.151	9.681	55.925	10.720	-1.233
2000	6.003	52.556	47.414	10.285	55.834	8.342	-.912

Phase change: 429.78 K, melting point of In; $\Delta H° = 0.780$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 5.422 + 0.656\times10^{-3}T - 0.568\times10^{5}T^{-2}$

$H°- H^{\circ}_{298} = 5.422\times10^{-3}T + 0.328\times10^{-6}T^{2} + 0.568\times10^{2}T^{-1} - 1.836$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf° = 57.241 + 2.802\times10^{-3}T - 4.434\times10^{-6}T^{2} + 139.500T^{-1}$

$\Delta Gf° = 57.241 - 2.802\times10^{-3}T\ln T + 4.434\times10^{-6}T^{2} + 69.750T^{-1} - 10.781\times10^{-3}T$

429.78-2000 K: $\Delta Hf° = 57.601 - 1.545\times10^{-3}T + 0.338\times10^{-6}T^{2} + 73.800T^{-1}$

$\Delta Gf° = 57.601 + 1.545\times10^{-3}T\ln T - 0.338\times10^{-6}T^{2} + 36.900T^{-1} - 35.746\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from Hilsenrath (94).

$In_2O_3(c)$

Diindium Trioxide, Indium Sesquioxide

[Formation: $2In(c,l) + 1.5O_2(g) = In_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	24.000	24.900	24.900	0	-221.270	-198.537	145.530
300	24.074	25.049	24.902	.044	-221.270	-198.396	144.530
400	26.831	32.414	25.887	2.611	-221.096	-190.797	104.245
429.78	27.234	34.355	26.407	3.416	-221.033	-188.543	95.876
429.78	27.234	34.355	26.407	3.416	-222.593	-188.543	95.876
500	28.183	38.561	27.825	5.368	-222.403	-182.993	79.985
600	29.010	43.778	30.060	8.231	-222.077	-175.140	63.794
700	29.590	48.295	32.349	11.162	-221.713	-167.346	52.247
800	30.037	52.277	34.597	14.144	-221.324	-159.608	43.602
900	30.408	55.837	36.763	17.167	-220.914	-151.916	36.890
1000	30.731	59.057	38.833	20.224	-220.487	-144.273	31.530
1100	31.022	62.000	40.807	23.312	-220.048	-136.671	27.154
1200	31.293	64.711	42.688	26.428	-219.594	-129.112	23.514
1300	31.549	67.226	44.480	29.570	-219.126	-121.592	20.441
1400	31.793	69.573	46.189	32.737	-218.645	-114.106	17.812
1500	32.030	71.775	47.822	35.929	-218.148	-106.655	15.539
1600	32.261	73.849	49.385	39.143	-217.639	-99.240	13.555

*Heat capacity at 298 K estimated.

Phase change: 429.78 K, melting point of In; $\Delta H° = 0.780$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp° = 29.323 + 1.936\times10^{-3}T - 5.245\times10^{5}T^{-2}$

$H°- H°_{298} = 29.323\times10^{-3}T + 0.968\times10^{-6}T^2 + 5.245\times10^{2}T^{-1} - 10.588$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf° = -226.476 + 13.238\times10^{-3}T - 9.311\times10^{-6}T^2 + 622.100T^{-1}$

$\Delta Gf° = -226.476 - 13.238\times10^{-3}T\ln T + 9.311\times10^{-6}T^2 + 311.050T^{-1} + 162.858\times10^{-3}T$

429.78-1600 K: $\Delta Hf° = -225.756 + 4.544\times10^{-3}T + 0.234\times10^{-6}T^2 + 490.700T^{-1}$

$\Delta Gf° = -225.756 - 4.544\times10^{-3}T\ln T - 0.234\times10^{-6}T^2 + 245.350T^{-1} + 112.927\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (236). Heat capacity at 298 K estimated. High-temperature data based on Tsagareishvili (228).

Ir(c)

Iridium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$, kcal/mol
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	
298.15	5.996	8.481	8.481	0
300	6.000	8.518	8.481	.011
400	6.102	10.257	8.717	.616
500	6.228	11.632	9.168	1.232
600	6.362	12.779	9.676	1.862
700	6.500	13.770	10.191	2.505
800	6.640	14.647	10.694	3.162
900	6.783	15.438	11.179	3.833
1000	6.927	16.160	11.642	4.518
1100	7.073	16.827	12.083	5.218
1200	7.221	17.448	12.504	5.933
1300	7.370	18.032	12.907	6.663
1400	7.521	18.584	13.293	7.407
1500	7.675	19.108	13.663	8.167
1600	7.830	19.608	14.019	8.942
1700	7.987	20.088	14.363	9.733
1800	8.147	20.549	14.693	10.540
1900	8.310	20.994	15.013	11.363
2000	8.475	21.424	15.323	12.202

Phase change: 2716 K, melting point of Ir; ΔH° = 6.247 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 5.448 + 1.478\times10^{-3}T + 0.096\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.448\times10^{-3}T + 0.739\times10^{-6}T^2 - 0.096\times10^{2}T^{-1} - 1.658$

Sources: Low-temperature heat capacities and entropy at 298 K from Furukawa (72). High-temperature data based on Jaeger (103) and Kelley (119).

Ir(g)

Iridium (ideal monatomic gas)

[Formation: Ir(c) = Ir(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	46.241	46.241	0	159.000	147.742	-108.296
300	4.968	46.271	46.241	.009	158.998	147.672	-107.578
400	4.976	47.701	46.436	.506	158.890	143.912	-78.629
500	5.007	48.814	46.804	1.005	158.773	140.182	-61.273
600	5.075	49.733	47.218	1.509	158.647	136.475	-49.710
700	5.180	50.522	47.635	2.021	158.516	132.790	-41.458
800	5.314	51.222	48.040	2.546	158.384	129.124	-35.275
900	5.464	51.857	48.429	3.085	158.252	125.475	-30.469
1000	5.622	52.441	48.802	3.639	158.121	121.840	-26.628
1100	5.780	52.984	49.158	4.209	157.991	118.218	-23.488
1200	5.933	53.494	49.498	4.795	157.862	114.607	-20.872
1300	6.078	53.974	49.824	5.395	157.732	111.007	-18.662
1400	6.215	54.430	50.137	6.010	157.603	107.419	-16.769
1500	6.340	54.863	50.438	6.638	157.471	103.839	-15.129
1600	6.455	55.276	50.727	7.278	157.336	100.267	-13.696
1700	6.560	55.670	51.006	7.929	157.196	96.707	-12.432
1800	6.654	56.048	51.276	8.589	157.049	93.151	-11.310
1900	6.739	56.410	51.537	9.259	156.896	89.606	-10.307
2000	6.815	56.758	51.790	9.937	156.735	86.067	-9.405

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.175 + 1.408\times10^{-3}T + 0.332\times10^{5}T^{-2}$

$H°- H°_{298} = 4.175\times10^{-3}T + 0.704\times10^{-6}T^{2} - 0.332\times10^{2}T^{-1} - 1.196$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 159.462 - 1.273\times10^{-3}T - 0.035\times10^{-6}T^{2} - 23.600T^{-1}$

$\Delta Gf° = 159.462 + 1.273\times10^{-3}T\ln T + 0.035\times10^{-6}T^{2} - 11.800T^{-1} - 46.440\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). All other data from Hilsenrath (94).

K(c,1,g)

Potassium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	7.050	15.457	15.457	0
300	7.068	15.501	15.458	.013
336.35	7.696	16.353	15.509	.284
336.35	7.707	18.012	15.509	.842
400	7.528	19.332	16.015	1.327
500	7.336	20.990	16.850	2.070
600	7.203	22.315	17.655	2.796
700	7.128	23.419	18.402	3.512
800	7.112	24.369	19.089	4.224
900	7.155	25.208	19.724	4.936
1000	7.256	25.967	20.310	5.657
1043.7	7.326	26.280	20.554	5.976
1043.7	4.968	44.521	20.554	25.014
1100	4.968	44.782	21.787	25.294
1200	4.968	45.215	23.722	25.791
1300	4.969	45.612	25.391	26.287
1400	4.970	45.981	26.850	26.784
1500	4.972	46.324	28.137	27.281
1600	4.975	46.645	29.283	27.779
1700	4.980	46.946	30.313	28.276
1800	4.988	47.231	31.245	28.775
1900	4.999	47.501	32.094	29.274
2000	5.013	47.758	32.870	29.775
2100	5.033	48.003	33.585	30.277
2200	5.057	48.238	34.247	30.781
2300	5.087	48.463	34.860	31.288
2400	5.122	48.680	35.430	31.799
2500	5.164	48.890	35.965	32.313
2600	5.213	49.094	36.466	32.832
2700	5.270	49.291	36.937	33.356
2800	5.334	49.484	37.382	33.886
2900	5.407	49.673	37.803	34.423
3000	5.489	49.857	38.201	34.968

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, calculated boiling point to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1037 K, normal boiling point to equilbrium mixture of K(g) and K_2(g).

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-336.35 K: $Cp^\circ = 1.046 + 20.136\times10^{-3}T$

$H^\circ - H^\circ_{298} = 1.046\times10^{-3}T + 10.068\times10^{-6}T^2 - 1.207$

336.35-1043.7 K: $Cp^\circ = 6.845 + 0.232\times10^{-3}T + 0.886\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.845\times10^{-3}T + 0.116\times10^{-6}T^2 - 0.886\times10^{2}T^{-1} - 1.210$

1043.7-3000 K: $Cp^\circ = 4.507 + 0.244\times10^{-3}T + 2.256\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.507\times10^{-3}T + 0.122\times10^{-6}T^2 - 2.256\times10^{2}T^{-1} + 20.393$

Source: Data from JANAF (51).

K(g)

Potassium (ideal monatomic gas)

[Formation: K(c,1,g) = K(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	38.297	38.297	0	21.310	14.500	-10.629
300	4.968	38.327	38.297	.009	21.306	14.458	-10.533
336.35	4.968	38.895	38.332	.190	21.216	13.634	-8.859
336.35	4.968	38.895	38.332	.190	20.658	13.634	-8.859
400	4.968	39.757	38.492	.506	20.489	12.319	-6.731
500	4.968	40.865	38.859	1.003	20.243	10.305	-4.504
600	4.968	41.771	39.271	1.500	20.014	8.340	-3.038
700	4.968	42.537	39.686	1.996	19.794	6.411	-2.002
800	4.968	43.200	40.084	2.493	19.579	4.514	-1.233
900	4.968	43.786	40.464	2.990	19.364	2.644	-.642
1000	4.968	44.309	40.822	3.487	19.140	.798	-.174
1043.7	4.968	44.521	40.972	3.704	19.038	0	0
1043.7	4.968	44.521	40.972	3.704	0	0	0
1100	4.968	44.782	41.160	3.984	0	0	0
1200	4.968	45.215	41.481	4.481	0	0	0
1300	4.969	45.612	41.784	4.977	0	0	0
1400	4.970	45.981	42.071	5.474	0	0	0
1500	4.972	46.324	42.343	5.971	0	0	0
1600	4.975	46.645	42.602	6.469	0	0	0
1700	4.980	46.946	42.848	6.966	0	0	0
1800	4.988	47.231	43.084	7.465	0	0	0
1900	4.999	47.501	43.309	7.964	0	0	0
2000	5.013	47.758	43.526	8.465	0	0	0
2100	5.033	48.003	43.733	8.967	0	0	0
2200	5.057	48.238	43.933	9.471	0	0	0
2300	5.087	48.463	44.125	9.978	0	0	0
2400	5.122	48.680	44.310	10.489	0	0	0
2500	5.164	48.890	44.489	11.003	0	0	0
2600	5.213	49.094	44.662	11.522	0	0	0
2700	5.270	49.291	44.830	12.046	0	0	0
2800	5.334	49.484	44.993	12.576	0	0	0
2900	5.407	49.673	45.151	13.113	0	0	0
3000	5.489	49.857	45.304	13.658	0	0	0

Phase changes: 336.35 K, melting point of K; $\Delta H° = 0.558$ kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; $\Delta H° = 19.038$ kcal/mol of K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 4.922 + 0.056\times10^{-3}T + 0.027\times10^{5}T^{-2}$

$H°-H°_{298} = 4.922\times10^{-3}T + 0.028\times10^{-6}T^{2} - 0.027\times10^{2}T^{-1} - 1.461$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = 21.056 + 3.876\times10^{-3}T - 10.040\times10^{-6}T^{2} - 2.700T^{-1}$

$\Delta Gf° = 21.056 - 3.876\times10^{-3}T\ln T + 10.040\times10^{-6}T^{2} - 1.350T^{-1} - 2.882\times10^{-3}T$

336.35-1043.7 K: $\Delta Hf° = 21.059 - 1.923\times10^{-3}T - 0.088\times10^{-6}T^{2} + 85.900T^{-1}$

$\Delta Gf° = 21.059 + 1.923\times10^{-3}T\ln T + 0.088\times10^{-6}T^{2} + 42.950T^{-1} - 33.675\times10^{-3}T$

1043.7-3000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Source: Data from JANAF (51).

$K_2(g)$

Potassium (ideal diatomic gas)

[Formation: $2K(c,l,g) = K_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	9.057	59.666	59.666	0	30.374	21.802	-15.981
300	9.058	59.722	59.666	.017	30.365	21.749	-15.844
336.35	9.081	60.759	59.729	.347	30.153	20.717	-13.461
336.35	9.081	60.759	59.729	.347	29.037	20.717	-13.461
400	9.121	62.336	60.021	.926	28.646	19.177	-10.478
500	9.177	64.378	60.696	1.841	28.075	16.876	-7.376
600	9.230	66.056	61.454	2.761	27.543	14.687	-5.350
700	9.281	67.482	62.215	3.687	27.037	12.586	-3.930
800	9.332	68.725	62.954	4.617	26.543	10.553	-2.883
900	9.382	69.827	63.657	5.553	26.055	8.585	-2.085
1000	9.432	70.818	64.324	6.494	25.554	6.670	-1.458
1043.7	9.454	71.222	64.604	6.907	25.329	5.851	-1.225
1043.7	9.454	71.222	64.604	6.907	-12.747	5.851	-1.225
1100	9.482	71.720	64.956	7.440	-12.774	6.854	-1.362
1200	9.532	72.547	65.555	8.390	-12.818	8.642	-1.574
1300	9.581	73.312	66.123	9.346	-12.854	10.432	-1.754
1400	9.631	74.024	66.662	10.307	-12.887	12.226	-1.909
1500	9.680	74.690	67.175	11.272	-12.916	14.021	-2.043
1600	9.730	75.316	67.664	12.243	-12.941	15.817	-2.161
1700	9.779	75.907	68.132	13.218	-12.960	17.615	-2.264
1800	9.826	76.468	68.580	14.198	-12.978	19.411	-2.357
1900	9.878	77.001	69.009	15.184	-12.990	21.212	-2.440
2000	9.927	77.508	69.421	16.174	-13.002	23.014	-2.515
2100	9.976	77.994	69.818	17.169	-13.011	24.814	-2.582
2200	10.026	78.459	70.200	18.169	-13.019	26.618	-2.644
2300	10.075	78.906	70.569	19.174	-13.028	28.418	-2.700
2400	10.124	79.336	70.926	20.184	-13.040	30.218	-2.752
2500	10.174	79.750	71.270	21.199	-13.053	32.022	-2.799
2600	10.223	80.150	71.604	22.219	-13.071	33.828	-2.843
2700	10.272	80.537	71.928	23.244	-13.094	35.627	-2.884
2800	10.322	80.911	72.242	24.273	-13.125	37.435	-2.922
2900	10.371	81.274	72.547	25.308	-13.164	39.245	-2.958
3000	10.420	81.627	72.844	26.348	-13.214	41.047	-2.990

Phase changes: 336.35 K, melting point of K; $\Delta H°$ = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; $\Delta H°$ = 19.038 kcal/mol of K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 8.943 + 0.492\times10^{-3}T - 0.030\times10^{5}T^{-2}$

$H°- H°_{298} = 8.943\times10^{-3}T + 0.246\times10^{-6}T^{2} + 0.030\times10^{2}T^{-1} - 2.698$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = 30.089 + 6.851\times10^{-3}T - 19.890\times10^{-6}T^{2} + 3.000T^{-1}$

$\Delta Gf° = 30.089 - 6.851\times10^{-3}T\ln T + 19.890\times10^{-6}T^{2} + 1.500T^{-1} + 5.290\times10^{-3}T$

336.35-1043.7 K: $\Delta Hf° = 30.096 - 4.747\times10^{-3}T + 0.014\times10^{-6}T^{2} + 180.200T^{-1}$

$\Delta Gf° = 30.096 + 4.747\times10^{-3}T\ln T - 0.014\times10^{-6}T^{2} + 90.100T^{-1} - 56.297\times10^{-3}T$

1043.7-3000 K: $\Delta Hf° = -13.110 - 0.071\times1^{-3}T + 0.002\times10^{-6}T^{2} + 454.200T^{-1}$

$\Delta Gf° = -13.110 + 0.071\times10^{-3}T\ln T - 0.002\times10^{-6}T^{2} + 227.100T^{-1} + 17.462\times10^{-3}T$

Source: Data from JANAF (51).

KO(g)

Potassium Oxide (ideal gas)

[Formation: $K(c,l,g) + 0.5O_2(g) = KO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.600	56.863	56.863	0	17.000	11.960	-8.767
300	8.604	56.916	56.863	.016	16.997	11.929	-8.690
336.35	8.672	57.904	56.923	.330	16.911	11.320	-7.355
336.35	8.672	57.904	56.923	.330	16.353	11.320	-7.355
400	8.791	59.420	57.202	.887	16.198	10.381	-5.672
500	8.896	61.394	57.852	1.771	15.974	8.952	-3.913
600	8.966	63.022	58.580	2.665	15.765	7.569	-2.757
700	9.018	64.409	59.318	3.564	15.558	6.219	-1.942
800	9.060	65.616	60.031	4.468	15.352	4.898	-1.338
900	9.095	66.685	60.712	5.376	15.141	3.605	-.875
1000	9.128	67.645	61.358	6.287	14.917	2.334	-.510
1043.7	9.141	68.036	61.629	6.686	14.815	1.787	-.374
1043.7	9.141	68.036	61.629	6.686	-4.223	1.787	-.374
1100	9.158	68.516	61.970	7.201	-4.226	2.112	-.420
1200	9.186	69.314	62.549	8.118	-4.229	2.688	-.490
1300	9.213	70.050	63.098	9.038	-4.234	3.266	-.549
1400	9.239	70.734	63.619	9.961	-4.240	3.843	-.600
1500	9.264	71.372	64.115	10.886	-4.247	4.421	-.644
1600	9.289	71.971	64.587	11.814	-4.255	4.999	-.683
1700	9.313	72.535	65.039	12.744	-4.263	5.577	-.717
1800	9.338	73.068	65.470	13.676	-4.274	6.155	-.747
1900	9.362	73.573	65.883	14.611	-4.285	6.736	-.775
2000	9.386	74.054	66.280	15.549	-4.298	7.316	-.799

*All data estimated.

Phase changes: 336.35 K, melting poin of K; $\Delta H° = 0.558$ kcal/mol.
1043.7 K, boiling point of K to ideal gas; $\Delta H° = 19.038$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.914 + 0.246\times10^{-3}T - 0.344\times10^{5}T^{-2}$

$H°- H°_{298} = 8.914\times10^{-3}T + 0.123\times10^{-6}T^2 + 0.344\times10^{2}T^{-1} - 2.784$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = 16.599 + 4.253\times10^{-3}T - 10.196\times10^{-6}T^2 + 11.800T^{-1}$

$\Delta Gf° = 16.599 - 4.253\times10^{-3}T\ln T + 10.196\times10^{-6}T^2 + 5.900T^{-1} + 5.568\times10^{-3}T$

336.35-1043.7 K: $\Delta Hf° = 16.602 - 1.546\times10^{-3}T - 0.244\times10^{-6}T^2 + 100.400T^{-1}$

$\Delta Gf° = 16.602 + 1.546\times10^{-3}T\ln T + 0.244\times10^{-6}T^2 + 50.200T^{-1} - 25.226\times10^{-3}T$

1043.7-2000 K: $\Delta Hf° = -5.001 + 0.792\times10^{-3}T - 0.250\times10^{-6}T^2 + 237.400T^{-1}$

$\Delta Gf° = -5.001 - 0.792\times10^{-3}T\ln T + 0.250\times10^{-6}T^2 + 118.700T^{-1} + 11.654\times10^{-3}T$

Source: Data are those estimated by JANAF (51).

$KO_2(c)$

Potassium Dioxide, Potassium Superoxide

[Formation: $K(c,l) + O_2(g) = KO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.530	29.280	29.280	0	-68.000	-57.510	42.156
300*	18.564	29.395	29.282	.034	-67.992	-57.446	41.848
336.35	19.029	31.545	29.412	.717	-67.836	-56.177	36.502
336.35	19.029	31.545	29.412	.717	-68.394	-56.177	36.502
400	19.842	34.935	30.028	1.963	-68.087	-53.892	29.445
500	20.582	39.447	31.475	3.986	-67.538	-50.406	22.032
600	21.158	43.252	33.129	6.074	-66.931	-47.035	17.132
700	21.689	46.553	34.814	8.217	-66.282	-43.769	13.665
800	22.224	49.484	36.469	10.412	-65.597	-40.601	11.092

*Data above 298 K estimated.

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
865 K, melting point of KO_2; ΔH° = 3.2 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp^\circ = 19.649 + 3.460\times10^{-3}T - 1.912\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.649\times10^{-3}T + 1.730\times10^{-6}T^2 + 1.912\times10^{2}T^{-1} - 6.653$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -71.095 + 11.373\times10^{-3}T - 8.841\times10^{-6}T^2 + 146.000T^{-1}$

$\Delta Gf^\circ = -71.095 - 11.373\times10^{-3}T\ln T + 8.841\times10^{-6}T^2 + 73.000T^{-1} + 106.903\times10^{-3}T$

336.35-800 K: $\Delta Hf^\circ = -71.091 + 5.574\times10^{-3}T + 1.111\times10^{-6}T^2 + 234.600T^{-1}$

$\Delta Gf^\circ = -71.091 - 5.574\times10^{-3}T\ln T - 1.111\times10^{-6}T^2 + 117.300T^{-1} + 76.110\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on D'Orazio (49) and Gilles (76). Entropy at 298 K from Chase (31). Low-temperature heat capacities from Todd (221). High-temperature data estimated. Fusion data from Byker (21).

$K_2O(c)$

Dipotassium Oxide

[Formation: $2K(c,l,g) + 0.5O_2(g) = K_2O(c)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	17.800	24.380	24.380	0	-81.260	-72.006	52.781
300	17.828	24.490	24.380	.033	-81.260	-71.949	52.414
336.35	18.224	26.552	24.505	.688	-81.274	-70.820	46.016
336.35	18.224	26.552	24.505	.688	-82.390	-70.820	46.016
400	18.918	29.781	25.094	1.875	-82.401	-68.629	37.497
500	19.642	34.084	26.476	3.804	-82.323	-65.195	28.496
600	20.219	37.718	28.055	5.798	-82.159	-61.782	22.504
700	20.728	40.873	29.664	7.846	-81.932	-58.402	18.234
800	21.204	43.672	31.243	9.943	-81.658	-55.061	15.042
900	21.661	46.196	32.767	12.086	-81.346	-51.754	12.567
1000	22.108	48.502	34.227	14.275	-81.012	-48.485	10.596
1043.7	22.302	49.452	34.845	15.245	-80.862	-47.065	9.855
1043.7	22.302	49.452	34.845	15.245	-118.938	-47.065	9.855
1100	22.551	50.630	35.623	16.508	-118.473	-43.201	8.583

*All data estimated except enthalpy of formation at 298 K. K_2O decomposes above 1100 K.

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal gas ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 18.154 + 4.090\times10^{-3}T - 1.398\times10^{5}T^{-2}$

$H°- H°_{298} = 18.154\times10^{-3}T + 2.045\times10^{-6}T^{2} + 1.398\times10^{2}T^{-1} - 6.063$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -83.734 + 12.447\times10^{-3}T - 18.343\times10^{-6}T^{2} + 117.200T^{-1}$

$\Delta Gf° = -83.734 - 12.447\times10^{-3}T\ln T + 18.343\times10^{-6}T^{2} + 58.600T^{-1} + 104.123\times10^{-3}T$

336.35-1043.7 K: $\Delta Hf° = -83.727 + 0.849\times10^{-3}T + 1.561\times10^{-6}T^{2} + 294.400T^{-1}$

$\Delta Gf° = -83.727 - 0.849\times10^{-3}T\ln T - 1.561\times10^{-6}T^{2} + 147.200T^{-1} + 42.537\times10^{-3}T$

1043.7-1100 K: $\Delta Hf° = -126.933 + 5.525\times10^{-3}T + 1.549\times10^{-6}T^{2} + 568.400T^{-1}$

$\Delta Gf° = -126.933 - 5.525\times10^{-3}T\ln T - 1.549\times10^{-6}T^{2} + 284.200T^{-1} + 116.296\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Byker (21). All other data estimated.

$K_2O_2(c)$

Dipotassium Dioxide, Potassium Peroxide

[Formation: $2K(c,l) + O_2(g) = K_2O_2(c)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	22.900	26.310	26.310	0	-118.400	-102.416	75.072
300	22.944	26.452	26.312	.042	-118.397	-102.317	74.537
336.35	23.669	29.118	26.474	.889	-118.348	-100.372	65.218
336.35	23.669	29.118	26.474	.889	-119.464	-100.372	65.218
400	24.938	33.344	27.237	2.443	-119.334	-96.770	52.872
500	26.509	39.082	29.048	5.017	-118.977	-91.168	39.849
600	27.922	44.042	31.142	7.740	-118.461	-85.650	31.198
700	29.262	48.447	33.306	10.599	-117.812	-80.231	25.049

*All data except enthalpy of formation and entropy at 298 K estimated.

Phase changes: 336.35 K, melting point of K; $\Delta H° = 0.558$ kcal/mol.
683 K, melting point of K_2O_2.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 21.080 + 12.156\times10^{-3}T - 1.604\times10^{5}T^{-2}$

$H°- H°_{298} = 21.080\times10^{-3}T + 6.078\times10^{-6}T^{2} + 1.604\times10^{2}T^{-1} - 7.363$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -120.998 + 11.758\times10^{-3}T - 14.561\times10^{-6}T^{2} + 115.200T^{-1}$

$\Delta Gf° = -120.998 - 11.758\times10^{-3}T\ln T + 14.561\times10^{-6}T^{2} + 57.600T^{-1} + 124.325\times10^{-3}T$

336.35-700 K: $\Delta Hf° = -120.991 + 0.160\times10^{-3}T + 5.343\times10^{-6}T^{2} + 292.400T^{-1}$

$\Delta Gf° = -120.991 - 0.160\times10^{-3}T\ln T - 5.343\times10^{-6}T^{2} + 146.200T^{-1} + 62.738\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K and temperature of fusion from Byker (21). All other data estimated.

Kr(g)

Krypton

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	4.968	39.191	39.191	0
300	4.968	39.222	39.192	.009
400	4.968	40.651	39.386	.506
500	4.968	41.759	39.753	1.003
600	4.968	42.665	40.165	1.500
700	4.968	43.431	40.580	1.996
800	4.968	44.094	40.978	2.493
900	4.968	44.680	41.358	2.990
1000	4.968	45.203	41.716	3.487
1100	4.968	45.677	42.055	3.984
1200	4.968	46.109	42.376	4.480
1300	4.968	46.506	42.678	4.977
1400	4.968	46.875	42.965	5.474
1500	4.968	47.217	43.236	5.971
1600	4.968	47.538	43.495	6.468
1700	4.968	47.839	43.743	6.964
1800	4.968	48.123	43.978	7.461
1900	4.968	48.392	44.204	7.958
2000	4.968	48.647	44.419	8.455
2100	4.968	48.889	44.626	8.952
2200	4.968	49.120	44.825	9.448
2300	4.968	49.341	45.017	9.945
2400	4.968	49.552	45.201	10.442
2500	4.968	49.755	45.379	10.939
2600	4.968	49.950	45.552	11.436
2700	4.968	50.137	45.718	11.932
2800	4.968	50.318	45.879	12.429
2900	4.968	50.492	46.035	12.926
3000	4.968	50.661	46.187	13.423

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 4.968$

$H^\circ - H^\circ_{298} = 4.968 \times 10^{-3} T - 1.481$

Source: Data from JANAF (52).

La(c,1)

Lanthanum

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.480	13.600	13.600	0
300	6.480	13.640	13.600	.012
400	6.550	15.510	13.850	.664
500	6.600	16.980	14.338	1.321
550	6.620	17.610	14.609	1.651
550	6.500	17.770	14.609	1.738
600	6.640	18.340	14.895	2.067
700	6.930	19.390	15.469	2.745
800	7.240	20.330	16.014	3.453
900	7.560	21.200	16.541	4.193
1000	7.900	22.020	17.054	4.966
1100	8.250	22.790	17.542	5.773
1134	8.370	23.040	17.702	6.055
1134	9.480	23.700	17.702	6.801
1193	9.480	24.180	18.010	7.360
1193	8.200	25.420	18.010	8.841
1200	8.200	25.470	18.055	8.898
1300	8.200	26.120	18.645	9.718
1400	8.200	26.730	19.203	10.538
1500*	8.200	27.300	19.728	11.358
1600	8.200	27.830	20.219	12.178
1700	8.200	28.320	20.674	12.998
1800	8.200	28.790	21.113	13.818
1900	8.200	29.240	21.536	14.638
2000	8.200	29.660	21.931	15.458

*Data above 1400 K extrapolated.

Phase changes: 550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.
1134 K, β - γ transition point of La; ΔH° = 0.746 kcal/mol.
1193 K, melting point of La; ΔH° = 1.481 kcal/mol.
3730 K, boiling point of La; ΔH° = 98.9 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp^\circ = 6.585 + 0.100\times10^{-3}T - 0.120\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.585\times10^{-3}T + 0.050\times10^{-6}T^2 + 0.120\times10^{2}T^{-1} - 2.008$

550-1134 K: $Cp^\circ = 4.319 + 3.504\times10^{-3}T + 0.768\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.319\times10^{-3}T + 1.752\times10^{-6}T^2 - 0.768\times10^{2}T^{-1} - 1.028$

1134-1193 K: $Cp^\circ = 9.475$

$H^\circ - H^\circ_{298} = 9.475\times10^{-3}T - 3.944$

1193-2000 K: $Cp^\circ = 8.200$

$H^\circ - H^\circ_{298} = 8.200\times10^{-3}T - 0.942$

Source: Data from Hultgren (99) who extrapolated above 1400 K by assuming constant heat capacity.

La(g)

Lanthanum (ideal monatomic gas)

[Formation: La(c,1) = La(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.438	43.564	43.564	0	103.000	94.066	-68.952
300	5.447	43.597	43.564	.010	102.998	94.011	-68.486
400	5.894	45.228	43.783	.578	102.914	91.027	-49.734
500	6.219	46.580	44.210	1.185	102.864	88.064	-38.492
550	6.337	47.179	44.454	1.499	102.848	86.586	-34.406
550	6.337	47.179	44.454	1.499	102.761	86.586	-34.406
600	6.455	47.736	44.704	1.819	102.752	85.114	-31.003
700	6.666	48.747	45.211	2.475	102.730	82.180	-25.657
800	6.874	49.650	45.710	3.152	102.699	79.243	-21.648
900	7.073	50.471	46.194	3.849	102.656	76.312	-18.531
1000	7.248	51.226	46.660	4.566	102.600	73.394	-16.040
1100	7.390	51.924	47.108	5.298	102.525	70.478	-14.002
1134	7.426	52.150	47.255	5.550	102.495	69.486	-13.392
1134	7.426	52.150	47.255	5.550	101.749	69.486	-13.392
1193	7.490	52.528	47.508	5.990	101.630	67.809	-12.422
1193	7.490	52.528	47.508	5.990	100.149	67.809	-12.422
1200	7.497	52.572	47.537	6.042	100.144	67.622	-12.315
1300	7.571	53.175	47.947	6.796	100.078	64.906	-10.912
1400	7.618	53.738	48.341	7.556	100.018	62.207	-9.711
1500	7.644	54.264	48.718	8.319	99.961	59.515	-8.671
1600	7.657	54.758	49.081	9.084	99.906	56.821	-7.761
1700	7.660	55.222	49.428	9.850	99.852	54.119	-6.957
1800	7.658	55.660	49.762	10.616	99.798	51.432	-6.245
1900	7.653	56.074	50.084	11.381	99.743	48.758	-5.608
2000	7.648	56.467	50.394	12.146	99.688	46.074	-5.035

Phase changes: 550 K, α - β transition point of La; $\Delta H°$ = 0.087 kcal/mol.
1134 K, β - γ transition point of La; $\Delta H°$ = 0.746 kcal/mol.
1193 K, melting point of La; $\Delta H°$ = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.000 + 1.162\times10^{-3}T - 0.808\times10^{5}T^{-2}$

$H°- H°_{298} = 6.000\times10^{-3}T + 0.581\times10^{-6}T^{2} + 0.808\times10^{2}T^{-1} - 2.112$

Formation equations (kcal/mol):

298.15-550 K: $\Delta Hf° = 102.896 - 0.585\times10^{-3}T + 0.531\times10^{-6}T^{2} + 68.800T^{-1}$

$\Delta Gf° = 102.896 + 0.585\times10^{-3}T\ln T - 0.531\times10^{-6}T^{2} + 34.400T^{-1} - 33.178\times10^{-3}T$

550-1134 K: $\Delta Hf° = 101.917 + 1.681\times10^{-3}T - 1.171\times10^{-6}T^{2} + 157.600T^{-1}$

$\Delta Gf° = 101.917 - 1.681\times10^{-3}T\ln T + 1.171\times10^{-6}T^{2} + 78.800T^{-1} - 18.181\times10^{-3}T$

1134-1193 K: $\Delta Hf° = 104.832 - 3.475\times10^{-3}T + 0.581\times10^{-6}T^{2} + 80.800T^{-1}$

$\Delta Gf° = 104.832 + 3.475\times10^{-3}T\ln T - 0.581\times10^{-6}T^{2} + 40.400T^{-1} - 55.001\times10^{-3}T$

1193-2000 K: $\Delta Hf° = 101.830 - 2.200\times10^{-3}T + 0.581\times10^{-6}T^{2} + 80.800T^{-1}$

$\Delta Gf° = 101.830 + 2.200\times10^{-3}T\ln T - 0.581\times10^{-6}T^{2} + 40.400T^{-1} - 43.452\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). All other data from Hilsenrath (94).

$La_2O_3(c)$

Dilanthanum Trioxide, Lanthanum Sesquioxide

[Formation: $2La(c,l) + 1.5O_2(g) = La_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	26.000	30.430	30.430	0	-428.700	-407.747	298.883
300	26.051	30.591	30.431	.048	-428.695	-407.617	296.945
400	27.939	38.381	31.481	2.760	-428.353	-400.643	218.898
500	28.968	44.734	33.514	5.610	-427.913	-393.759	172.110
550	29.336	47.515	34.663	7.069	-427.676	-390.354	155.110
550	29.336	47.515	34.663	7.069	-427.850	-390.354	155.110
600	29.703	50.084	35.842	8.545	-427.603	-386.958	140.947
700	30.312	54.709	38.215	11.546	-427.125	-380.214	118.707
800	30.855	58.793	40.537	14.605	-426.678	-373.553	102.049
900	31.353	62.456	42.772	17.716	-426.269	-366.938	89.104
1000	31.812	65.784	44.910	20.874	-425.897	-360.356	78.755
1100	32.233	68.836	46.948	24.077	-425.567	-353.815	70.296
1134	32.363	69.819	47.619	25.175	-425.463	-351.602	67.762
1134	32.363	69.819	47.619	25.175	-426.955	-351.602	67.762
1193	32.589	71.466	48.757	27.092	-426.908	-347.682	63.692
1193	32.589	71.466	48.757	27.092	-429.870	-347.682	63.692
1200	32.616	71.657	48.890	27.320	-429.846	-347.196	63.232
1300	32.961	74.282	50.744	30.599	-429.491	-340.340	57.216
1400	33.272	76.736	52.514	33.911	-429.115	-333.490	52.059
1500	33.552	79.041	54.206	37.252	-428.719	-326.661	47.594
1600	33.811	81.215	55.827	40.620	-428.306	-319.868	43.691
1700	34.059	83.272	57.381	44.014	-427.875	-313.127	40.255
1800	34.310	85.226	58.875	47.432	-427.429	-306.384	37.200
1900	34.582	87.088	60.311	50.877	-426.965	-299.647	34.467
2000	34.895	88.870	61.695	54.350	-426.480	-292.962	32.013

Phase changes: 550 K, α - β transition point of La; $\Delta H°$ = 0.087 kcal/mol.
1134 K, β - γ transition point of La; $\Delta H°$ = 0.746 kcal/mol.
1193 K, melting point of La; $\Delta H°$ = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 28.617 + 3.400\times10^{-3}T - 3.228\times10^{5}T^{-2}$

$H°- H°_{298} = 28.617\times10^{-3}T + 1.700\times10^{-6}T^{2} + 3.228\times10^{2}T^{-1} - 9.766$

Formation equations (kcal/mol):

298.15-550 K: $\Delta Hf° = -430.922 + 4.602\times10^{-3}T + 0.845\times10^{-6}T^{2} + 231.000T^{-1}$

$\Delta Gf° = -430.922 - 4.602\times10^{-3}T\ln T - 0.845\times10^{-6}T^{2} + 115.500T^{-1} + 102.903\times10^{-3}T$

550-1134 K: $\Delta Hf° = -432.882 + 9.134\times10^{-3}T - 2.559\times10^{-6}T^{2} + 408.600T^{-1}$

$\Delta Gf° = -432.882 - 9.134\times10^{-3}T\ln T + 2.559\times10^{-6}T^{2} + 204.300T^{-1} + 132.898\times10^{-3}T$

1134-1193 K: $\Delta Hf° = -427.051 - 1.178\times10^{-3}T + 0.946\times10^{-6}T^{2} + 255.000T^{-1}$

$\Delta Gf° = -427.051 + 1.178\times10^{-3}T\ln T - 0.946\times10^{-6}T^{2} + 127.500T^{-1} + 59.259\times10^{-3}T$

1193-2000 K: $\Delta Hf° = -433.055 + 1.372\times10^{-3}T + 0.946\times10^{-6}T^{2} + 255.000T^{-1}$

$\Delta Gf° = -433.055 - 1.372\times10^{-3}T\ln T - 0.946\times10^{-6}T^{2} + 127.500T^{-1} + 82.357\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). Low-temperature heat capacities and entropy at 298 K from Justice (109). High-temperature data based on King (135).

Li(c,l,g)

Lithium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.887	6.954	6.954	0
300	5.896	6.990	6.954	.011
400	6.599	8.774	7.194	.632
453.7	6.934	9.627	7.427	.998
453.7	7.265	11.207	7.427	1.715
500	7.200	11.915	7.815	2.050
600	7.060	13.216	8.611	2.763
700	6.928	14.294	9.347	3.463
800	6.916	15.218	10.024	4.155
900	6.904	16.032	10.648	4.846
1000	6.892	16.759	11.223	5.536
1100	6.880	17.415	11.757	6.224
1200	6.868	18.013	12.253	6.912
1300	6.860	18.562	12.717	7.598
1400	6.840	19.070	13.154	8.283
1500	6.820	19.541	13.564	8.966
1600	6.800	19.981	13.952	9.647
1638	6.792	20.140	14.093	9.905
1638	4.970	41.605	14.093	45.065
1700	4.971	41.792	15.101	45.375
1800	4.974	42.076	16.592	45.872
1900	4.978	42.345	17.940	46.370
2000	4.983	42.601	19.167	46.868
2100	4.991	42.844	20.288	47.367
2200	5.001	43.076	21.319	47.866
2300	5.014	43.299	22.270	48.367
2400	5.031	43.513	23.151	48.869
2500	5.051	43.719	23.970	49.373
2600	5.074	43.917	24.733	49.879
2700	5.102	44.109	25.447	50.388
2800	5.134	44.295	26.116	50.900
2900	5.169	44.476	26.747	51.415
3000	5.209	44.652	27.341	51.934

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1638 K, calculated boiling point to ideal monatomic gas; ΔH° = 35.160 kcal/mol.
1620 K, normal boiling point to equilibrium mixture of Li(g) and Li_2(g).

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-453.7 K: $Cp^\circ = 1.699 + 10.916\times10^{-3}T + 0.830\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 1.699\times10^{-3}T + 5.458\times10^{-6}T^2 - 0.830\times10^{2}T^{-1} - 0.713$

453.7-1638 K: $Cp^\circ = 6.797 - 0.012\times10^{-3}T + 0.973\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.797\times10^{-3}T - 0.006\times10^{-6}T^2 - 0.973\times10^{2}T^{-1} - 1.153$

1638-3000 K: $Cp^\circ = 5.211 - 0.044\times10^{-3}T - 4.506\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.211\times10^{-3}T - 0.022\times10^{-6}T^2 + 4.506\times10^{2}T^{-1} + 36.313$

Source: Data from JANAF (51).

Li(g)

Lithium (ideal monatomic gas)

[Formation: Li(c,l,g) = Li(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	33.143	33.143	0	38.410	30.602	-22.431
300	4.968	33.174	33.144	.009	38.408	30.553	-22.257
400	4.968	34.603	33.338	.506	38.284	27.952	-15.272
453.7	4.968	35.229	33.526	.773	38.185	26.569	-12.798
453.7	4.968	35.229	33.526	.773	37.468	26.569	-12.798
500	4.968	35.712	33.706	1.003	37.363	25.464	-11.130
600	4.968	36.618	34.118	1.500	37.147	23.106	-8.416
700	4.968	37.384	34.533	1.996	36.943	20.780	-6.488
800	4.968	38.047	34.931	2.493	36.748	18.485	-5.050
900	4.968	38.632	35.310	2.990	36.554	16.214	-3.937
1000	4.968	39.156	35.669	3.487	36.361	13.964	-3.052
1100	4.968	39.629	36.007	3.984	36.170	11.735	-2.331
1200	4.968	40.061	36.327	4.481	35.979	9.521	-1.734
1300	4.968	40.459	36.631	4.977	35.789	7.323	-1.231
1400	4.968	40.827	36.917	5.474	35.601	5.141	-.803
1500	4.969	41.170	37.189	5.971	35.415	2.972	-.433
1600	4.970	41.491	37.449	6.468	35.231	.815	-.111
1638	4.970	41.608	37.544	6.657	35.160	0	0
1638	4.970	41.608	37.544	6.657	0	0	0
1700	4.971	41.792	37.695	6.965	0	0	0
1800	4.974	42.076	37.930	7.462	0	0	0
1900	4.978	42.345	38.156	7.960	0	0	0
2000	4.983	42.601	38.372	8.458	0	0	0
2100	4.991	42.844	38.579	8.957	0	0	0
2200	5.001	43.076	38.778	9.456	0	0	0
2300	5.014	43.299	38.970	9.957	0	0	0
2400	5.031	43.513	39.155	10.459	0	0	0
2500	5.051	43.719	39.334	10.963	0	0	0
2600	5.074	43.917	39.506	11.469	0	0	0
2700	5.102	44.109	39.673	11.978	0	0	0
2800	5.134	44.295	39.834	12.490	0	0	0
2900	5.169	44.476	39.992	13.005	0	0	0
3000	5.209	44.652	40.144	13.524	0	0	0

Phase changes: 453.7 K, melting point of Li; $\Delta H°$ = 0.717 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; $\Delta H°$ = 35.160 kcal/mol of Li.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 4.951 + 0.020\times10^{-3}T + 0.010\times10^{5}T^{-2}$

$H°- H°_{298} = 4.951\times10^{-3}T + 0.010\times10^{-6}T^{2} - 0.010\times10^{2}T^{-1} - 1.474$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = 37.650 + 3.252\times10^{-3}T - 5.448\times10^{-6}T^{2} + 82.000T^{-1}$

$\Delta Gf° = 37.650 - 3.252\times10^{-3}T\ln T + 5.448\times10^{-6}T^{2} + 41.000T^{-1} - 7.196\times10^{-3}T$

453.7-1638 K: $\Delta Hf° = 38.089 - 1.846\times10^{-3}T + 0.016\times10^{-6}T^{2} + 96.300T^{-1}$

$\Delta Gf° = 38.089 + 1.846\times10^{-3}T\ln T - 0.016\times10^{-6}T^{2} + 48.150T^{-1} - 36.907\times10^{-3}T$

1638-3000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Source: Data from JANAF (51).

$Li_2(g)$

Lithium (ideal diatomic gas)

[Formation: $2Li(c,1,g) = Li_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.662	47.050	47.050	0	50.400	40.519	-29.701
300	8.627	47.104	47.051	.016	50.394	40.457	-29.472
400	8.826	49.616	47.391	.890	50.026	37.199	-20.324
453.7	8.888	50.733	47.724	1.365	49.769	35.487	-17.094
453.7	8.888	50.733	47.724	1.365	48.335	35.487	-17.094
500	8.942	51.599	48.043	1.778	48.078	34.194	-14.946
600	9.022	53.236	48.774	2.677	47.551	31.469	-11.462
700	9.084	54.632	49.515	3.582	47.056	28.825	-9.000
800	9.136	55.848	50.232	4.493	46.583	26.253	-7.172
900	9.182	56.927	50.917	5.409	46.117	23.740	-5.765
1000	9.224	57.897	51.567	6.330	45.658	21.279	-4.650
1100	9.264	58.778	52.183	7.254	45.206	18.863	-3.748
1200	9.301	59.585	52.767	8.182	44.758	16.487	-3.003
1300	9.338	60.331	53.320	9.114	44.318	14.149	-2.379
1400	9.374	61.025	53.846	10.050	43.884	11.845	-1.849
1500	9.409	61.673	54.347	10.989	43.457	9.571	-1.394
1600	9.444	62.281	54.823	11.932	43.038	7.328	-1.001
1638	9.457	62.503	54.999	12.291	42.881	6.480	-.865
1638	9.457	62.503	54.999	12.291	-27.439	6.480	-.865
1700	9.478	62.855	55.280	12.878	-27.472	7.767	-.999
1800	9.512	63.397	55.715	13.827	-27.517	9.842	-1.195
1900	9.546	63.913	56.134	14.780	-27.560	11.916	-1.371
2000	9.579	64.403	56.535	15.736	-27.600	13.998	-1.530
2100	9.612	64.871	56.921	16.696	-27.638	16.078	-1.673
2200	9.646	65.319	57.292	17.659	-27.673	18.160	-1.804
2300	9.679	65.749	57.651	18.625	-27.709	20.244	-1.924
2400	9.712	66.161	57.996	19.595	-27.743	22.333	-2.034
2500	9.745	66.558	58.331	20.567	-27.779	24.421	-2.135
2600	9.778	66.941	58.655	21.543	-27.815	26.507	-2.228
2700	9.810	67.311	58.969	22.523	-27.853	28.596	-2.315
2800	9.843	67.668	59.273	23.506	-27.894	30.688	-2.395
2900	9.876	68.014	59.568	24.492	-27.938	32.782	-2.471
3000	9.909	68.350	59.856	25.481	-27.987	34.875	-2.541

Phase changes: 453.7 K, melting point of Li; $\Delta H° = 0.717$ kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; $\Delta H° = 35.160$ kcal/mol of Li.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 8.896 + 0.346\times10^{-3}T - 0.300\times10^{5}T^{-2}$

$H°- H°_{298} = 8.896\times10^{-3}T + 0.173\times10^{-6}T^{2} + 0.300\times10^{2}T^{-1} - 2.768$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = 49.058 + 5.498\times10^{-3}T - 10.743\times10^{-6}T^{2} + 196.000T^{-1}$

$\Delta Gf° = 49.058 - 5.498\times10^{-3}T\ln T + 10.743\times10^{-6}T^{2} + 98.000T^{-1} - 1.622\times10^{-3}T$

453.7-1638 K: $\Delta Hf° = 49.938 - 4.698\times10^{-3}T + 0.185\times10^{-6}T^{2} + 224.600T^{-1}$

$\Delta Gf° = 49.938 + 4.698\times10^{-3}T\ln T - 0.185\times10^{-6}T^{2} + 112.300T^{-1} - 61.045\times10^{-3}T$

1638-3000 K: $\Delta Hf° = -24.995 - 1.526\times10^{-3}T + 0.217\times10^{-6}T^{2} - 871.200T^{-1}$

$\Delta Gf° = -24.995 + 1.526\times10^{-3}T\ln T - 0.217\times10^{-6}T^{2} - 435.600T^{-1} + 8.434\times10^{-3}T$

Source: Data from JANAF (51).

LiO(g)

Lithium Oxide (ideal gas)

[Formation: $Li(c,l,g) + 0.5O_2(g) = LiO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.745	50.395	50.395	0	20.100	14.453	-10.595
300	7.754	50.443	50.396	.014	20.097	14.418	-10.503
400	8.142	52.730	50.705	.810	19.917	12.552	-6.858
453.7	8.281	53.767	51.007	1.252	19.798	11.569	-5.573
453.7	8.281	53.767	51.007	1.252	19.081	11.569	-5.573
500	8.400	54.577	51.301	1.638	18.961	10.810	-4.725
600	8.573	56.125	51.978	2.488	18.721	9.204	-3.353
700	8.694	57.456	52.669	3.351	18.495	7.635	-2.384
800	8.782	58.623	53.342	4.225	18.278	6.098	-1.666
900	8.848	59.661	53.987	5.107	18.062	4.589	-1.114
1000	8.901	60.596	54.601	5.995	17.846	3.104	-.678
1100	8.945	61.447	55.186	6.887	17.631	1.640	-.326
1200	8.981	62.227	55.741	7.783	17.415	0.195	-.035
1300	9.013	62.947	56.268	8.683	17.201	-1.232	.207
1400	9.042	63.616	56.769	9.586	16.987	-2.641	.412
1500	9.067	64.241	57.247	10.491	16.774	-4.037	.588
1600	9.091	64.827	57.703	11.399	16.562	-5.416	.740
1638	9.099	65.040	57.870	11.745	16.482	-5.938	.792
1638	9.099	65.040	57.870	11.745	-18.678	-5.938	.792
1700	9.113	65.378	58.137	12.309	-18.697	-5.452	.701
1800	9.133	65.900	58.554	13.222	-18.725	-4.672	.567
1900	9.153	66.394	58.954	14.136	-18.756	-3.891	.448
2000	9.172	66.864	59.338	15.052	-18.787	-3.107	.340

Phase changes: 453.7 K, melting point of Li; $\Delta H° = 0.717$ kcal/mol.
1638 K, boiling point of Li to ideal gas; $\Delta H° = 35.160$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.547 + 0.390\times10^{-3}T - 0.816\times10^{5}T^{-2}$

$H°- H°_{298} = 8.547\times10^{-3}T + 0.195\times10^{-6}T^{2} + 0.816\times10^{2}T^{-1} - 2.839$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = 19.150 + 3.233\times10^{-3}T - 5.514\times10^{-6}T^{2} + 142.000T^{-1}$

$\Delta Gf° = 19.150 - 3.233\times10^{-3}T\ln T + 5.514\times10^{-6}T^{2} + 71.000T^{-1} + 0.225\times10^{-3}T$

453.7-1638 K: $\Delta Hf° = 19.590 - 1.865\times10^{-3}T - 0.050\times10^{-6}T^{2} + 156.300T^{-1}$

$\Delta Gf° = 19.590 + 1.865\times10^{-3}T\ln T + 0.050\times10^{-6}T^{2} + 78.150T^{-1} - 29.486\times10^{-3}T$

1638-2000 K: $\Delta Hf° = -17.877 - 0.279\times10^{-3}T - 0.034\times10^{-6}T^{2} - 391.600T^{-1}$

$\Delta Gf° = -17.877 + 0.279\times10^{-3}T\ln T + 0.034\times10^{-6}T^{2} - 195.800T^{-1} + 5.254\times10^{-3}T$

Source: Data from JANAF (51).

$Li_2O(c)$

Dilithium Oxide

[Formation: $2Li(c,l,g) + 0.5O_2(g) = Li_2O(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.930	9.056	9.056	0	-142.900	-134.148	98.332
300	12.988	9.136	9.056	.024	-142.904	-134.094	97.686
400	15.246	13.221	9.599	1.449	-143.076	-131.128	71.644
453.7	15.983	15.195	10.145	2.291	-143.161	-129.523	62.391
453.7	15.983	15.195	10.145	2.291	-144.595	-129.523	62.391
500	16.618	16.779	10.687	3.046	-144.681	-127.975	55.937
600	17.668	19.905	11.968	4.762	-144.768	-124.623	45.393
700	18.545	22.697	13.306	6.574	-144.745	-121.268	37.861
800	19.297	25.223	14.639	8.467	-144.635	-117.921	32.214
900	19.944	27.534	15.945	10.430	-144.462	-114.591	27.826
1000	20.502	29.665	17.212	12.453	-144.232	-111.284	24.321
1100	20.990	31.643	18.436	14.528	-143.952	-108.002	21.458
1200	21.430	33.488	19.613	16.650	-143.630	-104.748	19.077
1300	21.843	35.220	20.748	18.813	-143.268	-101.524	17.067
1400	22.250	36.854	21.841	21.018	-142.865	-98.327	15.349
1500	22.668	38.403	22.894	23.264	-142.419	-95.161	13.865
1600	23.104	39.880	23.910	25.552	-141.932	-92.026	12.570
1638	23.275	40.424	24.287	26.433	-141.734	-90.845	12.121
1638	23.275	40.424	24.287	26.433	-212.054	-90.845	12.121
1700	23.553	41.294	24.891	27.885	-211.496	-86.262	11.090
1800	23.995	42.653	25.840	30.263	-210.556	-78.922	9.582

Phase changes: 453.7 K, melting point of Li; $\Delta H° = 0.717$ kcal/mol.
1638 K, boiling point of Li to ideal gas; $\Delta H° = 35.160$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 15.813 + 4.870\times10^{-3}T - 3.854\times10^{5}T^{-2}$

$H°- H°_{298} = 15.813\times10^{-3}T + 2.435\times10^{-6}T^{2} + 3.854\times10^{2}T^{-1} - 6.224$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -146.521 + 8.800\times10^{-3}T - 8.733\times10^{-6}T^{2} + 528.800T^{-1}$

$\Delta Gf° = -146.521 - 8.800\times10^{-3}T\ln T + 8.733\times10^{-6}T^{2} + 264.400T^{-1} + 86.061\times10^{-3}T$

453.7-1638 K: $\Delta Hf° = -145.642 - 1.396\times10^{-3}T + 2.195\times10^{-6}T^{2} + 557.400T^{-1}$

$\Delta Gf° = -145.642 - 1.396\times10^{-3}T\ln T - 2.195\times10^{-6}T^{2} + 278.700T^{-1} + 26.637\times10^{-3}T$

1638-1800 K: $\Delta Hf° = -220.574 + 1.776\times10^{-3}T + 2.227\times10^{-6}T^{2} - 538.400T^{-1}$

$\Delta Gf° = -220.574 - 1.776\times10^{-3}T\ln T - 2.227\times10^{-6}T^{2} - 269.200T^{-1} + 96.117\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (104). Low-temperature heat capacities and entropy at 298 K from Johnston (107). High-temperature data based on Shomate (199).

$Li_2O_2(c)$

Dilithium Dioxide, Lithium Peroxide

[Formation: $2Li(c,l) + O_2(g) = Li_2O_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	19.297	13.500	13.500	0	-151.700	-136.968	100.399
300	19.304	13.619	13.500	.036	-151.699	-136.876	99.713
400	19.972	19.253	14.263	1.996	-151.691	-131.937	72.086
453.7	20.507	21.798	15.007	3.081	-151.728	-129.288	62.278
453.7	20.507	21.798	15.007	3.081	-153.162	-129.288	62.278
500	20.969	23.813	15.731	4.041	-153.213	-126.844	55.443
570	21.770	26.611	16.899	5.536	-153.245	-123.149	47.217

*Entropy at 298 K estimated. Decomposes above 570 K.

Phase change: 453.7 K, melting point of Li; $\Delta H° = 0.717$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-570 K: $Cp° = 14.266 + 12.462\times10^{-3}T + 1.170\times10^{5}T^{-2}$

$H°- H°_{298} = 14.266\times10^{-3}T + 6.231\times10^{-6}T^{2} - 1.170\times10^{2}T^{-1} - 4.415$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -152.336 + 3.638\times10^{-3}T - 5.188\times10^{-6}T^{2} + 3.800T^{-1}$

$\Delta Gf° = -152.336 - 3.638\times10^{-3}T\ln T + 5.188\times10^{-6}T^{2} + 1.900T^{-1} + 70.707\times10^{-3}T$

453.7-570 K: $\Delta Hf° = -151.457 - 6.558\times10^{-3}T + 5.740\times10^{-6}T^{2} + 32.400T^{-1}$

$\Delta Gf° = -151.457 + 6.558\times10^{-3}T\ln T - 5.740\times10^{-6}T^{2} + 16.200T^{-1} + 11.283\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from NBS (230). Entropy at 298 K estimated. High-temperature data based on Tanifuji (216).

Lu(c,l)

Lutetium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.400	12.180	12.180	0
300	6.400	12.220	12.180	.012
400	6.420	14.060	12.428	.653
500	6.460	15.500	12.906	1.297
600	6.500	16.680	13.438	1.945
700	6.610	17.690	13.977	2.599
800	6.790	18.590	14.504	3.269
900	7.000	19.400	15.002	3.958
1000	7.240	20.150	15.480	4.670
1100	7.530	20.850	15.934	5.408
1200	7.850	21.520	16.373	6.176
1300	8.220	22.160	16.791	6.980
1400	8.640	22.790	17.203	7.822
1500	9.090	23.400	17.595	8.707
1600	9.580	24.000	17.975	9.640
1700	10.110	24.590	18.341	10.623
1800	10.680	25.190	18.711	11.663
1900	11.250	25.780	19.064	12.761
1936	11.450	25.990	19.187	13.169
1936*	11.450	28.290	19.187	17.626
2000	11.450	28.670	19.493	18.355

*Enthalpy and entropy of fusion and data for Lu(1) estimated.

Phase changes: 1936 K, melting point of Lu; ΔH° = 4.457 kcal/mol.
3668 K, boiling point of Lu; ΔH° = 85.1 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1936 K: $Cp^\circ = 3.897 + 3.508\times10^{-3}T + 1.295\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 3.897\times10^{-3}T + 1.754\times10^{-6}T^{2} - 1.295\times10^{2}T^{-1} - 0.883$

1936-2000 K: $Cp^\circ = 11.450$

$H^\circ - H^\circ_{298} = 11.450\times10^{-3}T - 4.541$

Source: Data from Hultgren (99) who estimated enthalpy and entropy of fusion and data for Lu(1).

Lu(g)

Lutetium (ideal monatomic gas)

[Formation: Lu(c,1) = Lu(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.986	44.142	44.142	0	102.200	92.671	-67.928
300	4.987	44.172	44.142	.009	102.197	92.611	-67.466
400	5.085	45.618	44.338	.512	102.059	89.436	-48.865
500	5.282	46.772	44.712	1.030	101.933	86.297	-37.720
600	5.530	47.757	45.140	1.570	101.825	83.179	-30.297
700	5.773	48.628	45.577	2.136	101.737	80.080	-25.002
800	5.977	49.413	46.009	2.723	101.654	76.996	-21.034
900	6.129	50.126	46.427	3.329	101.571	73.918	-17.949
1000	6.231	50.778	46.830	3.948	101.478	70.850	-15.484
1100	6.292	51.375	47.217	4.574	101.366	67.788	-13.468
1200	6.320	51.924	47.586	5.205	101.229	64.744	-11.791
1300	6.325	52.430	47.940	5.837	101.057	61.706	-10.374
1400	6.314	52.898	48.277	6.469	100.847	58.696	-9.163
1500	6.294	53.333	48.600	7.100	100.593	55.693	-8.114
1600	6.268	53.738	48.908	7.728	100.288	52.707	-7.199
1700	6.239	54.118	49.204	8.353	99.930	49.732	-6.393
1800	6.209	54.473	49.486	8.976	99.513	46.804	-5.683
1900	6.179	54.808	49.758	9.595	99.034	43.881	-5.047
1936	6.169	54.924	49.853	9.817	98.848	42.830	-4.835
1936	6.169	54.924	49.853	9.817	94.391	42.830	-4.835
2000	6.150	55.124	50.019	10.211	94.056	41.148	-4.496

Phase change: 1936 K, melting point of Lu; $\Delta H° = 4.457$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 5.400 + 0.622\times10^{-3}T - 0.533\times10^{5}T^{-2}$

$H°- H°_{298} = 5.400\times10^{-3}T + 0.311\times10^{-6}T^{2} + 0.533\times10^{2}T^{-1} - 1.816$

Formation equations (kcal/mol):

298.15-1936 K: $\Delta Hf° = 101.267 + 1.503\times10^{-3}T - 1.443\times10^{-6}T^{2} + 182.800T^{-1}$

$\Delta Gf° = 101.267 - 1.503\times10^{-3}T\ln T + 1.443\times10^{-6}T^{2} + 91.400T^{-1} - 21.728\times10^{-3}T$

1936-2000 K: $\Delta Hf° = 104.925 - 6.050\times10^{-3}T + 0.311\times10^{-6}T^{2} + 53.300T^{-1}$

$\Delta Gf° = 104.925 + 6.050\times10^{-3}T\ln T - 0.311\times10^{-6}T^{2} + 26.650T^{-1} - 77.368\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). All other data from Feber (58).

$Lu_2O_3(c)$

Dilutetium Trioxide, Lutetium Sesquioxide

[Formation: $2Lu(c,l) + 1.5O_2(g) = Lu_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.320	26.281	26.281	0	-448.900	-427.556	313.403
300	24.390	26.432	26.282	.045	-448.898	-427.424	311.374
400	26.832	33.840	27.275	2.626	-448.664	-420.298	229.637
500	27.946	39.960	29.218	5.371	-448.304	-413.243	180.626
600	28.635	45.120	31.450	8.202	-447.901	-406.270	147.982
700	29.169	49.575	33.728	11.093	-447.486	-399.361	124.685
800	29.639	53.501	35.960	14.033	-447.083	-392.507	107.227
900	30.071	57.017	38.107	17.019	-446.695	-385.710	93.662
1000	30.469	60.207	40.161	20.046	-446.333	-378.955	82.819
1100	30.829	63.128	42.117	23.112	-446.001	-372.239	73.956
1200	31.143	65.824	43.981	26.211	-445.711	-365.541	66.573
1300	31.406	68.327	45.759	29.338	-445.475	-358.879	60.332
1400	31.615	70.663	47.456	32.490	-445.303	-352.208	54.981
1500	31.773	72.850	49.077	35.660	-445.208	-345.564	50.348
1600	31.886	74.904	50.627	38.843	-445.207	-338.928	46.295
1700	31.965	76.840	52.113	42.036	-445.303	-332.302	42.720
1800	32.029	78.669	53.538	45.235	-445.516	-325.629	39.536
1900	32.099	80.402	54.906	48.442	-445.846	-318.973	36.690
1936	32.137	81.005	55.386	49.598	-445.990	-316.582	35.738
1936	32.137	81.005	55.386	49.598	-454.904	-316.582	35.738
2000	32.204	82.051	56.223	51.657	-455.167	-311.971	34.090

Phase change: 1936 K, melting point of Lu; $\Delta H° = 4.457$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 28.552 + 2.298\times10^{-3}T - 4.371\times10^{5}T^{-2}$

$H°- H°_{298} = 28.552\times10^{-3}T + 1.149\times10^{-6}T^{2} + 4.371\times10^{2}T^{-1} - 10.081$

Formation equations (kcal/mol):

298.15-1936 K: $\Delta Hf° = -453.686 + 9.913\times10^{-3}T - 3.114\times10^{-6}T^{2} + 628.300T^{-1}$

$\Delta Gf° = -453.686 - 9.913\times10^{-3}T\ln T + 3.114\times10^{-6}T^{2} + 314.150T^{-1} + 139.657\times10^{-3}T$

1936-2000 K: $\Delta Hf° = -446.370 - 5.193\times10^{-3}T + 0.395\times10^{-6}T^{2} + 369.300T^{-1}$

$\Delta Gf° = -446.370 + 5.193\times10^{-3}T\ln T - 0.395\times10^{-6}T^{2} + 184.650T^{-1} + 28.376\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). Low-temperature heat capacities and entropy at 298 K from Justice (112). High-temperature data based on Pankratz (176) and Yashvili (253).

Mg(c,l,g)

Magnesium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.950	7.810	7.810	0
300	5.960	7.850	7.813	.011
400	6.240	9.600	8.048	.621
500	6.520	11.020	8.500	1.260
600	6.800	12.240	9.030	1.926
700	7.080	13.310	9.567	2.620
800	7.360	14.270	10.093	3.342
900	7.640	15.160	10.612	4.093
922	7.710	15.340	10.719	4.261
922	7.680	17.660	10.719	6.400
1000	7.880	18.290	11.280	7.010
1100	8.140	19.050	11.950	7.810
1200	8.400	19.770	12.570	8.640
1300	8.660	20.460	13.160	9.490
1363	8.820	20.860	13.491	10.040
1363	4.968	43.051	13.491	40.290
1400	4.968	43.185	14.275	40.474
1500	4.968	43.527	16.213	40.971
1600	4.968	43.848	17.931	41.468
1700	4.968	44.149	19.464	41.965
1800	4.968	44.433	20.844	42.461
1900	4.968	44.702	22.093	42.958
2000	4.969	44.957	23.229	43.455

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-922 K: $Cp^\circ = 5.143 + 2.776\times10^{-3}T - 0.019\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.143\times10^{-3}T + 1.388\times10^{-6}T^2 + 0.019\times10^{2}T^{-1} - 1.663$

922-1363 K: $Cp^\circ = 6.009 + 2.148\times10^{-3}T - 2.636\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.009\times10^{-3}T + 1.074\times10^{-6}T^2 + 2.636\times10^{2}T^{-1} - 0.339$

1363-2000 K: $Cp^\circ = 4.968$

$H^\circ - H^\circ_{298} = 4.968\times10^{-3}T + 33.519$

Sources: Data for Mg(c) and enthalpy of formation and entropy at 298 K for Mg(g) from Hultgren (99). Other data for Mg(g) from Hilsenrath (94). Data for Mg(l) based on Stull (213).

Mg(g)

Magnesium (ideal monatomic gas)

[Formation: Mg(c,l,g) = Mg(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	35.501	35.501	0	35.000	26.744	-19.604
300	4.968	35.532	35.502	.009	34.998	26.693	-19.446
400	4.968	36.961	35.696	.506	34.885	23.941	-13.080
500	4.968	38.069	36.063	1.003	34.743	21.219	-9.274
600	4.968	38.975	36.475	1.500	34.574	18.533	-6.751
700	4.968	39.741	36.890	1.996	34.376	15.874	-4.956
800	4.968	40.404	37.288	2.493	34.151	13.244	-3.618
900	4.968	40.990	37.668	2.990	33.897	10.650	-2.586
922	4.968	41.110	37.748	3.099	33.838	10.078	-2.389
922	4.968	41.110	37.748	3.099	31.699	10.078	-2.389
1000	4.968	41.513	38.026	3.487	31.477	8.254	-1.804
1100	4.968	41.987	38.365	3.984	31.174	5.943	-1.181
1200	4.968	42.419	38.685	4.481	30.841	3.662	-.667
1300	4.968	42.817	38.989	4.977	30.487	1.423	-.239
1363	4.968	43.052	39.171	5.290	30.250	0	0
1363	4.968	43.052	39.171	5.290	0	0	0
1400	4.968	43.185	39.275	5.474	0	0	0
1500	4.968	43.527	39.546	5.971	0	0	0
1600	4.968	43.848	39.806	6.468	0	0	0
1700	4.968	44.149	40.052	6.965	0	0	0
1800	4.968	44.433	40.288	7.461	0	0	0
1900	4.968	44.702	40.514	7.958	0	0	0
2000	4.969	44.957	40.729	8.455	0	0	0

Phase changes: 922 K, melting point of Mg; $\Delta H° = 2.139$ kcal/mol.
1363 K, boiling point of Mg; $\Delta H° = 30.250$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.968$

$H°-H°_{298} = 4.968\times10^{-3}T - 1.481$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = 35.182 - 0.175\times10^{-3}T - 1.388\times10^{-6}T^2 - 1.900T^{-1}$

$\Delta Gf° = 35.182 + 0.175\times10^{-3}T\ln T + 1.388\times10^{-6}T^2 - 0.950T^{-1} - 29.701\times10^{-3}T$

922-1363 K: $\Delta Hf° = 33.858 - 1.041\times10^{-3}T - 1.074\times10^{-6}T^2 - 263.600T^{-1}$

$\Delta Gf° = 33.858 + 1.041\times10^{-3}T\ln T + 1.074\times10^{-6}T^2 - 131.800T^{-1} - 33.734\times10^{-3}T$

1363-2000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Sources: Enthalpy of formation and entropy at 298 K from Hultgren (99). All other data from Hilsenrath (94).

$Mg_2(g)$

Magnesium (ideal diatomic gas)

[Formation: $2Mg(c,l,g) = Mg_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.658	58.282	58.282	0	68.590	55.870	-40.954
300	7.651	58.330	58.283	.014	68.582	55.793	-40.645
400	7.376	60.489	58.579	.764	68.112	51.596	-28.191
500	7.233	62.118	59.130	1.494	67.564	47.525	-20.773
600	7.151	63.428	59.741	2.212	66.950	43.581	-15.874
700	7.100	64.527	60.348	2.925	66.275	39.740	-12.407
800	7.066	65.472	60.931	3.633	65.539	35.993	-9.833
900	7.043	66.303	61.483	4.338	64.742	32.357	-7.857
922	7.039	66.473	61.600	4.493	64.561	31.560	-7.481
922	7.039	66.473	61.600	4.493	60.283	31.560	-7.481
1000	7.026	67.044	62.002	5.042	59.612	29.148	-6.370
1100	7.014	67.713	62.491	5.744	58.714	26.140	-5.193
1200	7.005	68.323	62.952	6.445	57.755	23.215	-4.228
1300	6.997	68.884	63.388	7.145	56.755	20.402	-3.430
1363	6.993	69.215	63.650	7.585	56.095	18.616	-2.985
1363	6.993	69.215	63.650	7.585	-4.405	18.616	-2.985
1400	6.991	69.402	63.799	7.844	-4.514	19.241	-3.004
1500	6.987	69.884	64.189	8.543	-4.809	20.946	-3.052
1600	6.983	70.335	64.559	9.242	-5.104	22.674	-3.097
1700	6.980	70.758	64.911	9.940	-5.400	24.418	-3.139
1800	6.977	71.157	65.247	10.638	-5.694	26.182	-3.179
1900	6.975	71.534	65.568	11.335	-5.991	27.962	-3.216
2000	6.973	71.892	65.876	12.032	-6.288	29.756	-3.252

Phase changes: 922 K, melting point of Mg; $\Delta H° = 2.139$ kcal/mol.
1363 K, boiling point of Mg; $\Delta H° = 30.250$ kcal/mol of Mg.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.011 - 0.034\times10^{-3}T + 0.585\times10^{5}T^{-2}$

$H°- H°_{298} = 7.011\times10^{-3}T - 0.017\times10^{-6}T^{2} - 0.585\times10^{2}T^{-1} - 1.893$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = 70.024 - 3.275\times10^{-3}T - 2.793\times10^{-6}T^{2} - 62.300T^{-1}$

$\Delta Gf° = 70.024 + 3.275\times10^{-3}T\ln T + 2.793\times10^{-6}T^{2} - 31.150T^{-1} - 66.613\times10^{-3}T$

922-1363 K: $\Delta Hf° = 67.376 - 5.007\times10^{-3}T - 2.165\times10^{-6}T^{2} - 585.700T^{-1}$

$\Delta Gf° = 67.376 + 5.007\times10^{-3}T\ln T + 2.165\times10^{-6}T^{2} - 292.850T^{-1} - 74.678\times10^{-3}T$

1363-2000 K: $\Delta Hf° = -0.339 - 2.925\times10^{-3}T - 0.017\times10^{-6}T^{2} - 58.500T^{-1}$

$\Delta Gf° = -0.339 + 2.925\times10^{-3}T\ln T + 0.017\times10^{-6}T^{2} - 29.250T^{-1} - 7.185\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (180). All other data from Chase (32).

MgO(c)

Magnesium Oxide, Periclase

[Formation: $Mg(c,l,g) + 0.5O_2(g) = MgO(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.882	6.440	6.440	0	-143.760	-136.046	99.723
300	8.915	6.495	6.442	.016	-143.761	-135.998	99.073
400	10.169	9.251	6.806	.978	-143.764	-133.407	72.889
500	10.848	11.598	7.538	2.030	-143.717	-130.826	57.183
600	11.285	13.616	8.386	3.138	-143.652	-128.249	46.714
700	11.604	15.381	9.262	4.283	-143.590	-125.687	39.241
800	11.856	16.947	10.126	5.457	-143.537	-123.135	33.639
900	12.057	18.355	10.964	6.652	-143.501	-120.582	29.281
922	12.095	18.647	11.144	6.918	-143.493	-120.026	28.451
922	12.095	18.647	11.144	6.918	-145.632	-120.026	28.451
1000	12.232	19.635	11.768	7.867	-145.616	-117.866	25.759
1100	12.382	20.808	12.537	9.098	-145.605	-115.094	22.867
1200	12.507	21.891	13.272	10.343	-145.613	-112.322	20.456
1300	12.586	22.895	13.974	11.597	-145.637	-109.535	18.414
1363	12.635	23.492	14.401	12.392	-145.664	-107.804	17.286
1363	12.635	23.492	14.401	12.392	-175.914	-107.804	17.286
1400	12.664	23.831	14.645	12.860	-175.790	-105.958	16.541
1500	12.743	24.707	15.287	14.130	-175.452	-100.983	14.713
1600	12.821	25.532	15.901	15.409	-175.109	-96.028	13.117
1700	12.900	26.312	16.491	16.695	-174.761	-91.097	11.711
1800	12.978	27.052	17.059	17.988	-174.408	-86.186	10.464
1900	13.057	27.755	17.602	19.290	-174.050	-81.293	9.351
2000	13.136	28.427	18.127	20.600	-173.686	-76.420	8.351

Phase changes: 922 K, melting point of Mg; $\Delta H°$ = 2.139 kcal/mol.
1363 K, boiling point of Mg; $\Delta H°$ = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.357 + 1.030\times10^{-3}T - 2.473\times10^{5}T^{-2}$

$H°- H°_{298} = 11.357\times10^{-3}T + 0.515\times10^{-6}T^{2} + 2.473\times10^{2}T^{-1} - 4.261$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -145.182 + 2.599\times10^{-3}T - 1.124\times10^{-6}T^{2} + 222.800T^{-1}$

$\Delta Gf° = -145.182 - 2.599\times10^{-3}T\ln T + 1.124\times10^{-6}T^{2} + 111.400T^{-1} + 43.862\times10^{-3}T$

922-1363 K: $\Delta Hf° = -146.506 + 1.733\times10^{-3}T - 0.810\times10^{-6}T^{2} - 38.900T^{-1}$

$\Delta Gf° = -146.506 - 1.733\times10^{-3}T\ln T + 0.810\times10^{-6}T^{2} - 19.450T^{-1} + 39.829\times10^{-3}T$

1363-2000 K: $\Delta Hf° = -180.363 + 2.774\times10^{-3}T + 0.264\times10^{-6}T^{2} + 224.700T^{-1}$

$\Delta Gf° = -180.363 - 2.774\times10^{-3}T\ln T - 0.264\times10^{-6}T^{2} + 112.350T^{-1} + 73.576\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (36). Low-temperature heat capacities and entropy at 298 K from Barron (11). High-temperature data based on Pankratz (177) and Victor (235).

MgO(g)

Magnesium Oxide (ideal gas)

[Formation: $Mg(c,l,g) + 0.5O_2(g) = MgO(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.689	50.946	50.946	0	13.900	8.344	-6.117
300	7.699	50.993	50.946	.014	13.896	8.311	-6.054
400	8.313	53.288	51.255	.813	13.730	6.473	-3.537
500	9.186	55.231	51.859	1.686	13.599	4.674	-2.043
600	10.296	57.002	52.570	2.659	13.528	2.900	-1.056
700	11.421	58.675	53.325	3.745	13.532	1.130	-.353
800	12.323	60.262	54.093	4.935	13.600	-.649	.177
900	12.880	61.749	54.862	6.198	13.705	-2.431	.590
922	12.928	62.061	55.030	6.482	13.731	-2.830	.671
922	12.928	62.061	55.030	6.482	11.592	-2.830	.671
1000	13.096	63.120	55.620	7.500	11.677	-4.058	.887
1100	13.051	64.368	56.360	8.809	11.766	-5.639	1.120
1200	12.841	65.496	57.075	10.105	11.808	-7.226	1.316
1300	12.547	66.512	57.763	11.374	11.800	-8.800	1.479
1363	12.342	67.101	58.181	12.159	11.762	-9.816	1.574
1363	12.342	67.101	58.181	12.159	-18.488	-9.816	1.574
1400	12.222	67.430	58.421	12.613	-18.377	-9.583	1.496
1500	11.903	68.262	59.049	13.819	-18.104	-8.966	1.306
1600	11.605	69.021	59.650	14.994	-17.864	-8.366	1.143
1700	11.338	69.716	60.221	16.141	-17.655	-7.778	1.000
1800	11.103	70.358	60.767	17.263	-17.473	-7.202	.874
1900	10.898	70.952	61.287	18.363	-17.317	-6.634	.763
2000	10.722	71.507	61.785	19.444	-17.182	-6.076	.664

Phase changes: 922 K, melting point of Mg; $\Delta H° = 2.139$ kcal/mol.
1363 K, boiling point of Mg; $\Delta H° = 30.250$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.495 + 1.464\times10^{-3}T - 2.883\times10^{5}T^{-2}$

$H°- H°_{298} = 10.495\times10^{-3}T + 0.732\times10^{-6}T^{2} + 2.883\times10^{2}T^{-1} - 4.161$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = 12.578 + 1.737\times10^{-3}T - 0.907\times10^{-6}T^{2} + 263.800T^{-1}$

$\Delta Gf° = 12.578 - 1.737\times10^{-3}T\ln T + 0.907\times10^{-6}T^{2} + 131.900T^{-1} - 6.057\times10^{-3}T$

922-1363 K: $\Delta Hf° = 11.254 + 0.871\times10^{-3}T - 0.593\times10^{-6}T^{2} + 2.100T^{-1}$

$\Delta Gf° = 11.254 - 0.871\times10^{-3}T\ln T + 0.593\times10^{-6}T^{2} + 1.050T^{-1} - 10.090\times10^{-3}T$

1363-2000 K: $\Delta Hf° = -22.603 + 1.912\times10^{-3}T + 0.481\times10^{-6}T^{2} + 265.700T^{-1}$

$\Delta Gf° = -22.603 - 1.912\times10^{-3}T\ln T - 0.481\times10^{-6}T^{2} + 132.850T^{-1} + 23.657\times10^{-3}T$

Source: Data from Chase (32).

Mn(c,l)

Manganese

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.280	7.650	7.650	0
300	6.290	7.690	7.650	.012
400	6.760	9.560	7.900	.664
500	7.210	11.120	8.396	1.362
600	7.630	12.470	8.963	2.104
700	8.010	13.670	9.547	2.886
800	8.350	14.760	10.130	3.704
900	8.650	15.760	10.700	4.554
980	8.850	16.510	11.147	5.254
980	8.980	17.050	11.147	5.786
1000	9.010	17.230	11.264	5.966
1100	9.110	18.100	11.854	6.871
1200	9.210	18.890	12.401	7.787
1300	9.320	19.630	12.928	8.713
1360	9.370	20.060	13.239	9.274
1360	10.300	20.430	13.239	9.781
1400	10.380	20.730	13.448	10.195
1410	10.400	20.810	13.506	10.299
1410	10.810	21.130	13.506	10.748
1500	10.990	21.800	13.981	11.729
1517	11.020	21.930	14.075	11.916
1517*	11.000	23.830	14.075	14.798
1600	11.000	24.420	14.601	15.711
1700	11.000	25.090	15.201	16.811
1800	11.000	25.720	15.769	17.911
1900	11.000	26.310	16.304	19.011
2000	11.000	26.880	16.824	20.111

*Enthalpy and entropy of fusion and data for Mn(1) estimated.

Phase changes: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.
2335 K, boiling point of Mn; ΔH° = 54.0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-980 K: $Cp^\circ = 5.638 + 3.414\times10^{-3}T - 0.334\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.638\times10^{-3}T + 1.707\times10^{-6}T^2 + 0.334\times10^{2}T^{-1} - 1.945$

980-1360 K: $Cp^\circ = 7.819 + 1.128\times10^{-3}T + 0.534\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.819\times10^{-3}T + 0.564\times10^{-6}T^2 - 0.534\times10^{2}T^{-1} - 2.364$

1360-1410 K: $Cp^\circ = 7.590 + 2.000\times10^{-3}T$

$H^\circ - H^\circ_{298} = 7.590\times10^{-3}T + 1.000\times10^{-6}T^2 - 2.391$

1410-1517 K: $Cp^\circ = 8.179 + 1.870\times10^{-3}T$

$H^\circ - H^\circ_{298} = 8.179\times10^{-3}T + 0.935\times10^{-6}T^2 - 2.643$

1517-2000 K: $Cp^\circ = 11.000$

$H^\circ - H^\circ_{298} = 11.000\times10^{-3}T - 1.889$

Source: Data from Hultgren (99) who estimated enthalpy and entropy of fusion and data for Mn(1).

Mn(g)

Manganese (ideal monatomic gas)

[Formation: Mn(c,l) = Mn(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	4.968	41.493	41.493	0	67.100	57.010	-41.789
300	4.968	41.523	41.493	.009	67.097	56.947	-41.485
400	4.968	42.953	41.688	.506	66.942	53.585	-29.277
500	4.968	44.061	42.055	1.003	66.741	50.270	-21.973
600	4.968	44.967	42.467	1.500	66.496	46.998	-17.119
700	4.968	45.733	42.882	1.996	66.210	43.766	-13.664
800	4.968	46.396	43.280	2.493	65.889	40.580	-11.086
900	4.968	46.981	43.659	2.990	65.536	37.437	-9.091
980	4.968	47.405	43.948	3.388	65.234	34.956	-7.795
980	4.968	47.405	43.948	3.388	64.702	34.956	-7.795
1000	4.968	47.505	44.018	3.487	64.621	34.346	-7.506
1100	4.968	47.978	44.356	3.984	64.213	31.347	-6.228
1200	4.968	48.410	44.677	4.480	63.793	28.369	-5.167
1300	4.968	48.808	44.980	4.977	63.364	25.433	-4.276
1360	4.968	49.032	45.153	5.275	63.101	23.697	-3.808
1360	4.968	49.032	45.153	5.275	62.594	23.697	-3.808
1400	4.968	49.176	45.266	5.474	62.379	22.555	-3.521
1410	4.968	49.211	45.294	5.524	62.325	22.280	-3.453
1410	4.968	49.211	45.294	5.524	61.876	22.280	-3.453
1500	4.968	49.519	45.538	5.971	61.342	19.763	-2.880
1517	4.968	49.575	45.583	6.055	61.239	19.302	-2.781
1517	4.968	49.575	45.583	6.055	58.357	19.302	-2.781
1600	4.969	49.840	45.798	6.468	57.857	17.185	-2.347
1700	4.969	50.141	46.044	6.965	57.254	14.667	-1.886
1800	4.971	50.425	46.279	7.462	56.651	12.182	-1.479
1900	4.973	50.694	46.505	7.959	56.048	9.718	-1.118
2000	4.977	50.949	46.721	8.456	55.445	7.307	-.798

Phase changes: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 4.968$

$H^\circ - H^\circ_{298} = 4.968 \times 10^{-3} T - 1.481$

Mn(g) - Continued

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf^\circ = 67.564 - 0.670\times10^{-3}T - 1.707\times10^{-6}T^2 - 33.400T^{-1}$

$\Delta Gf^\circ = 67.564 + 0.670\times10^{-3}T\ln T + 1.707\times10^{-6}T^2 - 16.700T^{-1} - 39.536\times10^{-3}T$

980-1360 K: $\Delta Hf^\circ = 67.983 - 2.851\times10^{-3}T - 0.564\times10^{-6}T^2 + 53.400T^{-1}$

$\Delta Gf^\circ = 67.983 + 2.851\times10^{-3}T\ln T + 0.564\times10^{-6}T^2 + 26.700T^{-1} - 53.911\times10^{-3}T$

1360-1410 K: $\Delta Hf^\circ = 68.010 - 2.622\times10^{-3}T - 1.000\times10^{-6}T^2$

$\Delta Gf^\circ = 68.010 + 2.622\times10^{-3}T\ln T + 1.000\times10^{-6}T^2 - 52.857\times10^{-3}T$

1410-1517 K: $\Delta Hf^\circ = 68.262 - 3.211\times10^{-3}T - 0.935\times10^{-6}T^2$

$\Delta Gf^\circ = 68.262 + 3.211\times10^{-3}T\ln T + 0.935\times10^{-6}T^2 - 57.215\times10^{-3}T$

1517-2000 K: $\Delta Hf^\circ = 67.508 - 6.032\times10^{-3}T$

$\Delta Gf^\circ = 67.508 + 6.032\times10^{-3}T\ln T - 75.962\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). All other data from Hilsenrath (94).

MnO(c)

Manganese Oxide

[Formation: Mn(c) + 0.5O_2(g) = MnO(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.540	14.270	14.270	0	-92.070	-86.738	63.580
300	10.559	14.335	14.270	.020	-92.070	-86.705	63.163
400	11.306	17.495	14.695	1.120	-91.975	-84.931	46.404
500	11.703	20.064	15.522	2.271	-91.888	-83.180	36.357
600	11.993	22.224	16.462	3.457	-91.822	-81.445	29.666
700	12.242	24.092	17.422	4.669	-91.781	-79.722	24.890
800	12.475	25.742	18.361	5.905	-91.761	-78.003	21.309
900	12.704	27.224	19.264	7.164	-91.759	-76.284	18.524
980	12.888	28.314	19.960	8.187	-91.767	-74.905	16.704
980	12.888	28.314	19.960	8.187	-92.299	-74.905	16.704
1000	12.934	28.575	20.130	8.445	-92.304	-74.554	16.294
1100	13.167	29.818	20.954	9.750	-92.324	-72.769	14.458
1200	13.403	30.974	21.742	11.079	-92.334	-70.998	12.930
1300	13.642	32.056	22.494	12.431	-92.337	-69.222	11.637
1360	13.787	32.675	22.930	13.254	-92.334	-68.147	10.951
1360	13.787	32.675	22.930	13.254	-92.841	-68.147	10.951
1400	13.883	33.076	23.214	13.807	-92.875	-67.422	10.525
1410	13.907	33.175	23.284	13.946	-92.883	-67.230	10.421
1410	13.907	33.175	23.284	13.946	-93.332	-67.230	10.421
1500	14.125	34.042	23.903	15.208	-93.442	-65.566	9.553

Phase changes: 980 K, α - β transition point of Mn; $\Delta H°$ = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; $\Delta H°$ = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; $\Delta H°$ = 0.449 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 11.215 + 1.858\times10^{-3}T - 1.092\times10^{5}T^{-2}$

$H°- H°_{298} = 11.215\times10^{-3}T + 0.929\times10^{-6}T^{2} + 1.092\times10^{2}T^{-1} - 3.793$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf° = -92.742 + 1.962\times10^{-3}T - 1.030\times10^{-6}T^{2} + 53.200T^{-1}$

$\Delta Gf° = -92.742 - 1.962\times10^{-3}T\ln T + 1.030\times10^{-6}T^{2} + 26.600T^{-1} + 30.709\times10^{-3}T$

980-1360 K: $\Delta Hf° = -92.323 - 0.219\times10^{-3}T + 0.113\times10^{-6}T^{2} + 140.000T^{-1}$

$\Delta Gf° = -92.323 + 0.219\times10^{-3}T\ln T - 0.113\times10^{-6}T^{2} + 70.000T^{-1} + 16.334\times10^{-3}T$

1360-1410 K: $\Delta Hf° = -92.296 + 0.010\times10^{-3}T - 0.322\times10^{-6}T^{2} + 86.600T^{-1}$

$\Delta Gf° = -92.296 - 0.010\times10^{-3}T\ln T + 0.322\times10^{-6}T^{2} + 43.300T^{-1} + 17.388\times10^{-3}T$

1410-1500 K: $\Delta Hf° = -92.043 - 0.579\times10^{-3}T - 0.257\times10^{-6}T^{2} + 86.600T^{-1}$

$\Delta Gf° = -92.043 + 0.579\times10^{-3}T\ln T + 0.257\times10^{-6}T^{2} + 43.300T^{-1} + 13.030\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). Low-temperature heat capacities and entropy at 298 K from Todd (223). High-temperature data based on Southard (208).

$MnO_2(c)$

Manganese Dioxide

[Formation: $Mn(c) + O_2(g) = MnO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.005	12.680	12.680	0	-124.290	-111.179	81.495
300	13.064	12.761	12.681	.024	-124.291	-111.098	80.934
400	15.173	16.847	13.222	1.450	-124.227	-106.706	58.301
500	16.250	20.360	14.308	3.026	-124.080	-102.340	44.732
600	16.920	23.386	15.576	4.686	-123.917	-98.008	35.699
700	17.399	26.032	16.885	6.403	-123.760	-93.706	29.256
800*	17.775	28.380	18.176	8.163	-123.616	-89.424	24.429

*Decomposes near 800 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 16.930 + 1.816\times10^{-3}T - 3.970\times10^{5}T^{-2}$

$H°- H°_{298} = 16.930\times10^{-3}T + 0.908\times10^{-6}T^{2} + 3.970\times10^{2}T^{-1} - 6.460$

Formation equations (kcal/mol):

298.15-800 K: $\Delta Hf° = -126.453 + 4.062\times10^{-3}T - 1.302\times10^{-6}T^{2} + 318.400T^{-1}$

$\Delta Gf° = -126.453 - 4.062\times10^{-3}T\ln T + 1.302\times10^{-6}T^{2} + 159.200T^{-1} + 72.195\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). Low-temperature heat capacities and entropy at 298 K from Kelley (123). High-temperature data based on Moore (160).

Mn_2O_3

Dimanganese Trioxide, Manganese Sesquioxide

[Formation: $2Mn(c) + 1.5O_2(g) = Mn_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	23.670	26.400	26.400	0	-229.200	-210.593	154.367
300	23.726	26.547	26.400	.044	-229.199	-210.478	153.331
400	26.026	33.715	27.363	2.541	-229.072	-204.256	111.599
500	27.588	39.699	29.249	5.225	-228.880	-198.069	86.575
600	28.847	44.843	31.428	8.049	-228.673	-191.927	69.908
700	29.953	49.374	33.674	10.990	-228.462	-185.825	58.017
800	30.966	53.441	35.896	14.036	-228.249	-179.754	49.106
900	31.918	57.144	38.054	17.181	-228.025	-173.706	42.181
980	32.643	59.893	39.725	19.764	-227.833	-168.880	37.661
980	32.643	59.893	39.725	19.764	-228.897	-168.880	37.661
1000	32.824	60.554	40.135	20.419	-228.852	-167.661	36.642
1100	33.693	63.723	42.137	23.745	-228.594	-161.536	32.094
1200	34.530	66.691	44.061	27.156	-228.287	-155.470	28.315
1300	35.338	69.487	45.910	30.650	-227.930	-149.419	25.119
1350	35.733	70.828	46.808	32.427	-227.734	-146.382	23.697

*Heat capacity at 298 K estimated.

Phase changes: 980 K, α - β transition point of Mn; $\Delta H° = 0.532$ kcal/mol.
1350 K, Mn_2O_3 decomposes above this temperature.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1350 K: $Cp° = 24.570 + 8.526\times10^{-3}T - 3.060\times10^{5}T^{-2}$

$H°- H°_{298} = 24.570\times10^{-3}T + 4.263\times10^{-6}T^{2} + 3.060\times10^{2}T^{-1} - 8.731$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf° = -230.513 + 2.449\times10^{-3}T + 0.095\times10^{-6}T^{2} + 171.400T^{-1}$

$\Delta Gf° = -230.513 - 2.449\times10^{-3}T\ln T - 0.095\times10^{-6}T^{2} + 85.700T^{-1} + 79.830\times10^{-3}T$

980-1350 K: $\Delta Hf° = -229.675 - 1.913\times10^{-3}T + 2.381\times10^{-6}T^{2} + 345.000T^{-1}$

$\Delta Gf° = -229.675 + 1.913\times10^{-3}T\ln T - 2.381\times10^{-6}T^{2} + 172.500T^{-1} + 51.081\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (237). High-temperature data based on Orr (172). Heat capacity at 298 K estimated since available low-temperature heat capacities disagree with those derived from high-temperature data by about 8 pct at 298 K.

$Mn_3O_4(c)$

Trimanganese Tetroxide

[Formation: $3Mn(c,l) + 2O_2(g) = Mn_3O_4(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	33.583	37.200	37.200	0	-331.700	-306.727	224.834
300	33.671	37.408	37.201	.062	-331.700	-306.572	223.335
400	37.532	47.662	38.572	3.636	-331.502	-298.223	162.939
500	39.980	56.323	41.279	7.522	-331.172	-289.932	126.728
600	41.401	63.751	44.421	11.598	-330.832	-281.720	102.615
700	42.146	70.195	47.654	15.779	-330.553	-273.568	85.411
800	42.556	75.852	50.832	20.016	-330.366	-265.448	72.516
900	42.967	80.886	53.896	24.291	-330.269	-257.340	62.490
980	43.564	84.565	56.252	27.747	-330.234	-250.850	55.941
980	43.564	84.565	56.252	27.747	-331.830	-250.850	55.941
1000	43.713	85.447	56.827	28.620	-331.830	-249.207	54.463
1100	45.128	89.673	59.623	33.055	-331.788	-240.920	47.866
1200	47.545	93.695	62.296	37.679	-331.608	-232.691	42.378
1300	51.298	97.639	64.863	42.609	-331.168	-224.468	37.736
1360	54.551	100.015	66.361	45.770	-330.726	-219.526	35.277
1360	54.551	100.015	66.361	45.770	-332.247	-219.526	35.277
1400	56.719	101.628	67.346	47.995	-331.956	-216.221	33.753
1410	57.402	102.034	67.590	48.566	-331.871	-215.366	33.381
1410	57.402	102.034	67.590	48.566	-333.218	-215.366	33.381
1445	59.792	103.469	68.441	50.615	-332.915	-212.440	32.130
1445	50.200	106.466	68.442	54.945	-328.585	-212.440	32.130
1500	50.200	108.341	69.870	57.706	-328.587	-208.040	30.311
1517	50.200	108.907	70.305	58.559	-328.592	-206.645	29.770
1517	50.200	108.907	70.305	58.559	-337.238	-206.645	29.770
1600	50.200	111.581	72.377	62.726	-337.267	-199.480	27.247
1700	50.200	114.625	74.774	67.746	-337.311	-190.851	24.535
1800	50.200	117.494	77.068	72.766	-337.367	-182.225	22.125

Phase changes: 980 K, α - β transition point of Mn; $\Delta H° = 0.532$ kcal/mol.
1360 K, β - γ transition point of Mn; $\Delta H° = 0.507$ kcal/mol.
1410 K, γ - δ transition point of Mn; $\Delta H° = 0.449$ kcal/mol.
1445 K, α - β transition point of Mn_3O_4; $\Delta H° = 4.330$ kcal/mol.
1517 K, melting point of Mn; $\Delta H° = 2.882$ kcal/mol.
1835 ± 5 K, melting point of Mn_3O_4.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1445 K: $Cp° = 35.046 + 11.592\times10^{-3}T - 4.372\times10^{5}T^{-2}$

$H°- H°_{298} = 35.046\times10^{-3}T + 5.796\times10^{-6}T^{2} + 4.372\times10^{2}T^{-1} - 12.431$

1445-1800 K: $Cp° = 50.200$

$H°- H°_{298} = 50.200\times10^{-3}T - 17.594$

Mn_3O_4(c) - Continued

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf° = -333.592 + 3.672\times10^{-3}T - 0.331\times10^{-6}T^2 + 246.600T^{-1}$

$\Delta Gf° = -333.592 - 3.672\times10^{-3}T\ln T + 0.331\times10^{-6}T^2 + 123.300T^{-1} + 109.543\times10^{-3}T$

980-1360 K: $\Delta Hf° = -332.335 - 2.871\times10^{-3}T + 3.098\times10^{-6}T^2 + 507.000T^{-1}$

$\Delta Gf° = -332.335 + 2.871\times10^{-3}T\ln T - 3.098\times10^{-6}T^2 + 253.500T^{-1} + 66.420\times10^{-3}T$

1360-1410 K: $\Delta Hf° = -332.254 - 2.184\times10^{-3}T + 1.790\times10^{-6}T^2 + 346.800T^{-1}$

$\Delta Gf° = -332.254 + 2.184\times10^{-3}T\ln T - 1.790\times10^{-6}T^2 + 173.400T^{-1} + 69.581\times10^{-3}T$

1410-1445 K: $\Delta Hf° = -331.497 - 3.951\times10^{-3}T + 1.985\times10^{-6}T^2 + 346.800T^{-1}$

$\Delta Gf° = -331.497 + 3.951\times10^{-3}T\ln T - 1.985\times10^{-6}T^2 + 173.400T^{-1} + 56.506\times10^{-3}T$

1445-1517 K: $\Delta Hf° = -336.660 + 11.203\times10^{-3}T - 3.811\times10^{-6}T^2 - 90.400T^{-1}$

$\Delta Gf° = -336.660 - 11.203\times10^{-3}T\ln T + 3.811\times10^{-6}T^2 - 45.200T^{-1} + 162.067\times10^{-3}T$

1517-1800 K: $\Delta Hf° = -338.922 + 2.740\times10^{-3}T - 1.006\times10^{-6}T^2 - 90.400T^{-1}$

$\Delta Gf° = -338.922 - 2.740\times10^{-3}T\ln T + 1.006\times10^{-6}T^2 - 45.200T^{-1} + 105.827\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (237). Low-temperature heat capacities from Millar (155). High-temperature data based on Southard (207).

Mo(c,l)

Molybdenum

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.750	6.850	6.850	0
300	5.752	6.886	6.850	.011
400	5.980	8.573	7.078	.598
500	6.164	9.928	7.518	1.205
600	6.315	11.066	8.016	1.830
700	6.436	12.049	8.525	2.467
800	6.539	12.915	9.020	3.116
900	6.636	13.691	9.497	3.775
1000	6.766	14.396	9.951	4.445
1100	6.912	15.048	10.385	5.129
1200	7.068	15.656	10.800	5.827
1300	7.229	16.228	11.196	6.542
1400	7.395	16.770	11.575	7.273
1500	7.570	17.286	11.938	8.022
1600	7.763	17.781	12.289	8.788
1700	7.975	18.258	12.626	9.575
1800	8.200	18.720	12.952	10.383
1900	8.447	19.170	13.267	11.216
2000	8.717	19.610	13.573	12.074
2100	9.006	20.042	13.871	12.959
2200	9.327	20.468	14.160	13.877
2300	9.692	20.891	14.445	14.825
2400	10.089	21.311	14.722	15.814
2500	10.517	21.731	14.993	16.845
2600	10.977	22.153	15.261	17.920
2700	11.462	22.576	15.524	19.041
2800	11.982	23.002	15.783	20.212
2890	12.500	23.389	16.014	21.314
2890	8.190	26.080	16.014	29.091
2900	8.190	26.108	16.048	29.173
3000	8.190	26.386	16.389	29.992

Phase change: 2890 K, melting point of Mo; ΔH° = 7.777 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2890 K: $Cp^\circ = 4.377 + 2.370\times10^{-3}T + 0.592\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.377\times10^{-3}T + 1.185\times10^{-6}T^2 - 0.592\times10^{2}T^{-1} - 1.212$

2890-3000 K: $Cp^\circ = 8.190$

$H^\circ - H^\circ_{298} = 8.190\times10^{-3}T + 5.422$

Source: Data from Hultgren (99).

Mo(g)

Molybdenum (ideal monatomic gas)

[Formation: Mo(c,l) = Mo(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	43.461	43.461	0	157.500	146.584	-107.448
300	4.968	43.492	43.462	.009	157.498	146.516	-106.736
400	4.968	44.921	43.656	.506	157.408	142.869	-78.059
500	4.968	46.030	44.024	1.003	157.298	139.247	-60.864
600	4.968	46.935	44.435	1.500	157.170	135.649	-49.409
700	4.968	47.701	44.850	1.996	157.029	132.073	-41.234
800	4.968	48.365	45.249	2.493	156.877	128.517	-35.109
900	4.968	48.950	45.628	2.990	156.715	124.982	-30.349
1000	4.968	49.473	45.986	3.487	156.542	121.465	-26.546
1100	4.969	49.947	46.325	3.984	156.355	117.966	-23.437
1200	4.970	50.379	46.645	4.481	156.154	114.486	-20.851
1300	4.972	50.777	46.948	4.978	155.936	111.022	-18.664
1400	4.977	51.146	47.235	5.475	155.702	107.576	-16.793
1500	4.985	51.489	47.507	5.973	155.451	104.147	-15.174
1600	4.998	51.811	47.766	6.472	155.184	100.736	-13.760
1700	5.016	52.115	48.013	6.973	154.898	97.341	-12.514
1800	5.043	52.402	48.249	7.476	154.593	93.965	-11.409
1900	5.079	52.676	48.475	7.982	154.266	90.605	-10.422
2000	5.125	52.937	48.691	8.492	153.918	87.264	-9.536
2100	5.183	53.189	48.900	9.007	153.548	83.939	-8.736
2200	5.254	53.432	49.101	9.529	153.152	80.631	-8.010
2300	5.340	53.667	49.294	10.058	152.733	77.348	-7.350
2400	5.440	53.896	49.481	10.597	152.283	74.079	-6.746
2500	5.556	54.121	49.662	11.147	151.802	70.827	-6.192
2600	5.689	54.341	49.838	11.709	151.289	67.600	-5.682
2700	5.838	54.559	50.009	12.285	150.744	64.390	-5.212
2800	6.005	54.774	50.175	12.877	150.165	61.203	-4.777
2890	6.172	54.967	50.321	13.425	149.611	58.352	-4.413
2890	6.172	54.967	50.321	13.425	141.834	58.352	-4.413
2900	6.190	54.988	50.337	13.487	141.814	58.062	-4.376
3000	6.391	55.201	50.496	14.116	141.624	55.179	-4.020

Phase change: 2890 K, melting point of Mo; $\Delta H° = 7.777$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 4.748 + 0.222\times10^{-3}T + 0.137\times10^{5}T^{-2}$

$H°- H°_{298} = 4.748\times10^{-3}T + 0.111\times10^{-6}T^{2} - 0.137\times10^{2}T^{-1} - 1.380$

Formation equations (kcal/mol):

298.15-2890 K: $\Delta Hf° = 157.332 + 0.371\times10^{-3}T - 1.074\times10^{-6}T^{2} + 45.500T^{-1}$

$\Delta Gf° = 157.332 - 0.371\times10^{-3}T\ln T + 1.074\times10^{-6}T^{2} + 22.750T^{-1} - 34.511\times10^{-3}T$

2890-3000 K: $\Delta Hf° = 150.698 - 3.442\times10^{-3}T + 0.111\times10^{-6}T^{2} - 13.700T^{-1}$

$\Delta Gf° = 150.698 + 3.442\times10^{-3}T\ln T - 0.111\times10^{-6}T^{2} - 6.850T^{-1} - 59.173\times10^{-3}T$

Source: Data from JANAF (55).

MoO(g)

Molybdenum Oxide (ideal gas)

[Formation: $Mo(c) + 0.5O_2(g) = MoO(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.605	57.757	57.757	0	74.321	66.448	-48.707
300	8.607	57.810	57.757	.016	74.319	66.400	-48.371
400	8.694	60.301	58.096	.882	74.243	63.770	-34.842
500	8.740	62.246	58.738	1.754	74.143	61.164	-26.735
600	8.779	63.843	59.460	2.630	74.016	58.579	-21.337
700	8.814	65.199	60.186	3.509	73.869	56.018	-17.489
800	8.845	66.378	60.888	4.392	73.704	53.478	-14.609
900	8.871	67.421	61.557	5.278	73.524	50.961	-12.375
1000	8.893	68.357	62.191	6.166	73.329	48.463	-10.591
1100	8.912	69.205	62.790	7.056	73.116	45.987	-9.137
1200	8.928	69.981	63.358	7.948	72.885	43.532	-7.928
1300	8.943	70.697	63.895	8.842	72.637	41.095	-6.909
1400	8.956	71.360	64.405	9.737	72.368	38.680	-6.038
1500	8.968	71.978	64.889	10.633	72.081	36.282	-5.286
1600	8.979	72.557	65.350	11.531	71.774	33.908	-4.632
1700	8.989	73.102	65.791	12.429	71.444	31.550	-4.056
1800	8.998	73.616	66.212	13.328	71.091	29.214	-3.547
1900	9.007	74.103	66.614	14.229	70.712	26.897	-3.094
2000	9.015	74.565	67.000	15.130	70.305	24.601	-2.688

*All data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.724 + 0.170\times10^{-3}T - 0.151\times10^{5}T^{-2}$

$H°- H°_{298} = 8.724\times10^{-3}T + 0.085\times10^{-6}T^{2} + 0.151\times10^{2}T^{-1} - 2.659$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 74.049 + 0.732\times10^{-3}T - 1.351\times10^{-6}T^{2} + 51.700T^{-1}$

$\Delta Gf° = 74.049 - 0.732\times10^{-3}T\ln T + 1.351\times10^{-6}T^{2} + 25.850T^{-1} - 22.017\times10^{-3}T$

Source: Data from JANAF (56) who estimated all except enthalpy of formation at 298 K.

$MoO_2(c)$

Molybdenum Dioxide

[Formation: $Mo(c) + O_2(g) = MoO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.380	11.060	11.060	0	-140.760	-127.404	93.389
300	13.342	11.143	11.060	.025	-140.759	-127.321	92.752
400	15.143	15.261	11.611	1.460	-140.621	-122.860	67.127
500	16.249	18.766	12.700	3.033	-140.386	-118.444	51.771
600	17.087	21.806	13.969	4.702	-140.097	-114.083	41.554
700	17.787	24.493	15.284	6.446	-139.768	-109.772	34.272
800	18.404	26.910	16.590	8.256	-139.405	-105.513	28.824
900	18.970	29.110	17.860	10.125	-139.009	-101.299	24.598
1000	19.504	31.137	19.088	12.049	-138.582	-97.133	21.228
1100	20.021	33.020	20.269	14.026	-138.128	-93.008	18.479
1200	20.530	34.784	21.407	16.053	-137.647	-88.927	16.196
1300	21.041	36.447	22.499	18.132	-137.139	-84.887	14.271
1400	21.562	38.026	23.553	20.262	-136.604	-80.888	12.627
1500	22.101	39.531	24.568	22.444	-136.041	-76.929	11.208
1600	22.664	40.976	25.550	24.682	-135.446	-73.008	9.972
1700	23.261	42.367	26.498	26.978	-134.819	-69.122	8.886
1800	23.896	43.715	27.417	29.336	-134.157	-65.276	7.926
1900	24.576	45.025	28.310	31.759	-133.461	-61.470	7.071
2000	25.309	46.304	29.178	34.253	-132.724	-57.700	6.305

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.786 + 4.982\times10^{-3}T - 2.570\times10^{5}T^{-2}$

$H°- H°_{298} = 14.786\times10^{-3}T + 2.491\times10^{-6}T^{2} + 2.570\times10^{2}T^{-1} - 5.492$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -142.688 + 3.179\times10^{-3}T + 0.803\times10^{-6}T^{2} + 271.000T^{-1}$

$\Delta Gf° = -142.688 - 3.179\times10^{-3}T\ln T - 0.803\times10^{-6}T^{2} + 135.500T^{-1} + 68.090\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). Low-temperature heat capacities and entropy at 298 K from King (128). High-temperature data based on King (134).

$MoO_2(g)$

Molybdenum Dioxide (ideal gas)

[Formation: $Mo(c) + O_2(g) = MoO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.558	66.176	66.176	0	-1.987	-5.064	3.712
300	10.576	66.241	66.176	.020	-1.991	-5.083	3.703
400	11.454	69.410	66.603	1.123	-2.185	-6.084	3.324
500	12.090	72.038	67.434	2.302	-2.344	-7.039	3.076
600	12.531	74.284	68.394	3.534	-2.492	-7.965	2.901
700	12.840	76.240	69.377	4.804	-2.637	-8.863	2.767
800	13.060	77.970	70.345	6.100	-2.788	-9.744	2.662
900	13.221	79.518	71.280	7.414	-2.947	-10.604	2.575
1000	13.341	80.917	72.175	8.742	-3.116	-11.447	2.502
1100	13.434	82.193	73.028	10.081	-3.300	-12.270	2.438
1200	13.505	83.366	73.843	11.428	-3.499	-13.077	2.382
1300	13.562	84.449	74.617	12.782	-3.716	-13.866	2.331
1400	13.608	85.456	75.355	14.141	-3.952	-14.638	2.285
1500	13.646	86.396	76.061	15.503	-4.209	-15.395	2.243
1600	13.677	87.278	76.735	16.869	-4.486	-16.131	2.203
1700	13.703	88.108	77.379	18.239	-4.785	-16.848	2.166
1800	13.725	88.891	77.997	19.610	-5.110	-17.546	2.130
1900	13.743	89.634	78.590	20.983	-5.464	-18.230	2.097
2000	13.759	90.339	79.160	22.358	-5.846	-18.892	2.064

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.588 + 0.806\times10^{-3}T - 2.018\times10^{5}T^{-2}$

$H°- H°_{298} = 12.588\times10^{-3}T + 0.403\times10^{-6}T^2 + 2.018\times10^{2}T^{-1} - 4.466$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -2.889 + 0.981\times10^{-3}T - 1.285\times10^{-6}T^2 + 215.800T^{-1}$

$\Delta Gf° = -2.889 - 0.981\times10^{-3}T\ln T + 1.285\times10^{-6}T^2 + 107.900T^{-1} - 3.303\times10^{-3}T$

Source: Data from JANAF (56).

MoO_3(c,1)

Molybdenum Trioxide

[Formation: $Mo(c) + 1.5O_2(g) = MoO_3(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.920	18.580	18.580	0	-178.080	-159.661	117.033
300	17.971	18.691	18.581	.033	-178.077	-159.547	116.228
400	19.792	24.113	19.306	1.923	-177.839	-153.401	83.814
500	21.052	28.672	20.736	3.968	-177.498	-147.329	64.397
600	22.063	32.602	22.394	6.125	-177.098	-141.333	51.480
700	22.976	36.073	24.104	8.378	-176.649	-135.405	42.275
800	23.844	39.198	25.799	10.719	-176.155	-129.549	35.391
900	24.685	42.055	27.448	13.146	-175.608	-123.754	30.051
1000	25.500	44.698	29.043	15.655	-175.009	-118.026	25.794
1075	26.091	46.564	30.201	17.590	-174.528	-113.769	23.129
1075	30.170	57.438	30.201	29.280	-162.838	-113.769	23.129
1100	30.170	58.132	30.828	30.034	-162.573	-112.631	22.378
1200	30.170	60.757	33.215	33.051	-161.526	-108.136	19.694
1300	30.170	63.172	35.427	36.068	-160.508	-103.729	17.438
1400	30.170	65.408	37.490	39.085	-159.518	-99.399	15.517

Phase changes: 1075 K, melting point of MoO_3; $\Delta H° = 11.690$ kcal/mol.
1428 K, boiling point of MoO_3 to equilibrium mixture of polymeric species $(MoO_3)_x$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1075 K: $Cp° = 18.047 + 7.668\times10^{-3}T - 2.145\times10^{5}T^{-2}$

$H°- H°_{298} = 18.047\times10^{-3}T + 3.834\times10^{-6}T^{2} + 2.145\times10^{2}T^{-1} - 6.441$

1075-1400 K: $Cp° = 30.170$

$H°- H°_{298} = 30.170\times10^{-3}T - 3.153$

Formation equations (kcal/mol):

298.15-1075 K: $\Delta Hf° = -179.781 + 2.825\times10^{-3}T + 1.895\times10^{-6}T^{2} + 205.900T^{-1}$

$\Delta Gf° = -179.781 - 2.825\times10^{-3}T\ln T - 1.895\times10^{-6}T^{2} + 102.950T^{-1} + 82.986\times10^{-3}T$

1075-1400 K: $\Delta Hf° = -176.493 + 14.948\times10^{-3}T - 1.939\times10^{-6}T^{2} - 8.600T^{-1}$

$\Delta Gf° = -176.493 - 14.948\times10^{-3}T\ln T + 1.939\times10^{-6}T^{2} - 4.300T^{-1} + 160.518\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (237). Low-temperature heat capacities from Kelley (122). High-temperature data based on King (134).

$MoO_3(g)$

Molybdenum Trioxide (ideal gas)

[Formation: $Mo(c) + 1.5O_2(g) = MoO_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.192	67.827	67.827	0	-82.800	-79.064	57.955
300	14.225	67.915	67.828	.026	-82.805	-79.041	57.581
400	15.769	72.231	68.406	1.530	-82.953	-77.762	42.486
500	16.848	75.873	69.543	3.165	-83.021	-76.453	33.417
600	17.588	79.015	70.867	4.889	-83.055	-75.137	27.368
700	18.102	81.767	72.231	6.675	-83.073	-73.814	23.046
800	18.467	84.209	73.579	8.504	-83.090	-72.493	19.804
900	18.733	86.400	74.883	10.365	-83.109	-71.166	17.281
1000	18.933	88.385	76.136	12.249	-83.135	-69.839	15.263
1100	19.085	90.197	77.333	14.150	-83.177	-68.507	13.611
1200	19.204	91.863	78.476	16.064	-83.233	-67.171	12.233
1300	19.298	93.404	79.566	17.990	-83.306	-65.829	11.067
1400	19.374	94.837	80.606	19.923	-83.400	-64.482	10.066
1500	19.435	96.176	81.600	21.864	-83.513	-63.128	9.198
1600	19.487	97.432	82.551	23.810	-83.648	-61.764	8.436
1700	19.529	98.614	83.460	25.761	-83.807	-60.389	7.763
1800	19.565	99.732	84.334	27.716	-83.992	-59.006	7.164
1900	19.596	100.790	85.172	29.674	-84.208	-57.613	6.627
2000	19.662	101.796	85.979	31.635	-84.454	-56.207	6.142

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 17.812 + 1.216\times10^{-3}T - 3.541\times10^{5}T^{-2}$

$H°- H°_{298} = 17.812\times10^{-3}T + 0.608\times10^{-6}T^{2} + 3.541\times10^{2}T^{-1} - 6.552$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -84.613 + 2.590\times10^{-3}T - 1.332\times10^{-6}T^{2} + 345.500T^{-1}$

$\Delta Gf° = -84.613 - 2.590\times10^{-3}T\ln T + 1.332\times10^{-6}T^{2} + 172.750T^{-1} + 31.027\times10^{-3}T$

Source: Data from JANAF (56).

$N_2(g)$

Nitrogen

T, K	cal/mol•K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.961	45.770	45.770	0
300	6.961	45.813	45.770	.013
400	6.991	47.818	46.043	.710
500	7.070	49.386	46.560	1.413
600	7.196	50.685	47.142	2.126
700	7.350	51.806	47.730	2.853
800	7.513	52.798	48.303	3.596
900	7.670	53.692	48.853	4.355
1000	7.815	54.508	49.378	5.130
1100	7.945	55.259	49.879	5.918
1200	8.060	55.955	50.357	6.718
1300	8.161	56.605	50.813	7.529
1400	8.250	57.213	51.249	8.350
1500	8.328	57.785	51.666	9.179
1600	8.396	58.324	52.065	10.015
1700	8.456	58.835	52.448	10.858
1800	8.508	59.320	52.817	11.706
1900	8.555	59.781	53.171	12.559
2000	8.597	60.221	53.513	13.417
2100	8.634	60.641	53.841	14.279
2200	8.668	61.044	54.160	15.144
2300	8.699	61.430	54.468	16.012
2400	8.726	61.801	54.766	16.883
2500	8.751	62.157	55.054	17.757
2600	8.775	62.501	55.334	18.634
2700	8.796	62.833	55.606	19.512
2800	8.815	63.153	55.870	20.393
2900	8.833	63.463	56.127	21.275
3000	8.850	63.762	56.376	22.159

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 6.517 + 1.178\times10^{-3}T + 0.079\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.517\times10^{-3}T + 0.589\times10^{-6}T^2 - 0.079\times10^{2}T^{-1} - 1.969$

2000-3000 K: $Cp^\circ = 8.645 + 0.112\times10^{-3}T - 10.920\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.645\times10^{-3}T + 0.056\times10^{-6}T^2 + 10.920\times10^{2}T^{-1} - 4.643$

Source: Data from JANAF (52).

N(g)

Nitrogen (ideal monatomic gas)

[Formation: $0.5N_2(g) = N(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	36.613	36.613	0	112.970	108.877	-79.808
300	4.968	36.644	36.614	.009	112.973	108.851	-79.297
400	4.968	38.073	36.808	.506	113.121	107.455	-58.710
500	4.968	39.182	37.176	1.003	113.267	106.022	-46.342
600	4.968	40.088	37.588	1.500	113.407	104.560	-38.085
700	4.968	40.854	38.003	1.996	113.540	103.074	-32.181
800	4.968	41.517	38.401	2.493	113.665	101.571	-27.747
900	4.968	42.102	38.780	2.990	113.783	100.052	-24.296
1000	4.968	42.626	39.139	3.487	113.892	98.520	-21.531
1100	4.968	43.099	39.477	3.984	113.995	96.979	-19.268
1200	4.968	43.531	39.798	4.480	114.091	95.427	-17.379
1300	4.968	43.929	40.101	4.977	114.182	93.868	-15.780
1400	4.968	44.297	40.387	5.474	114.269	92.302	-14.409
1500	4.968	44.640	40.659	5.971	114.352	90.730	-13.219
1600	4.968	44.961	40.918	6.468	114.431	89.152	-12.177
1700	4.968	45.262	41.166	6.964	114.505	87.569	-11.258
1800	4.968	45.546	41.401	7.461	114.578	85.983	-10.440
1900	4.968	45.814	41.626	7.958	114.648	84.394	-9.707
2000	4.969	46.069	41.841	8.455	114.717	82.800	-9.048
2100	4.970	46.312	42.049	8.952	114.783	81.200	-8.451
2200	4.971	46.543	42.248	9.449	114.847	79.601	-7.908
2300	4.972	46.764	42.440	9.946	114.910	77.997	-7.411
2400	4.975	46.975	42.624	10.443	114.972	76.393	-6.956
2500	4.978	47.179	42.803	10.941	115.033	74.781	-6.537
2600	4.982	47.374	42.974	11.439	115.092	73.171	-6.150
2700	4.987	47.562	43.141	11.937	115.151	71.558	-5.792
2800	4.993	47.743	43.302	12.436	115.209	69.943	-5.459
2900	5.001	47.919	43.458	12.936	115.269	68.325	-5.149
3000	5.010	48.088	43.609	13.436	115.326	66.705	-4.859

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 4.968$

$H°- H°_{298} = 4.968\times10^{-3}T - 1.481$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 112.473 + 1.710\times10^{-3}T - 0.295\times10^{-6}T^2 + 3.950T^{-1}$

$\Delta Gf° = 112.473 - 1.710\times10^{-3}T\ln T + 0.295\times10^{-6}T^2 + 1.975T^{-1} - 2.432\times10^{-3}T$

2000-3000 K: $\Delta Hf° = 113.810 + 0.645\times10^{-3}T - 0.028\times10^{-6}T^2 - 546.000T^{-1}$

$\Delta Gf° = 113.810 - 0.645\times10^{-3}T\ln T + 0.028\times10^{-6}T^2 - 273.000T^{-1} - 10.586\times10^{-3}T$

Source: Data from JANAF (52).

NO(g)

Nitrogen Oxide (ideal gas), Nitric Oxide

[Formation: $0.5N_2(g) + 0.5O_2(g) = NO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.133	50.347	50.347	0	21.570	20.688	-15.164
300	7.132	50.392	50.349	.013	21.570	20.682	-15.066
400	7.157	52.444	50.626	.727	21.580	20.385	-11.137
500	7.287	54.053	51.157	1.448	21.584	20.085	-8.779
600	7.466	55.397	51.754	2.186	21.589	19.785	-7.207
700	7.655	56.562	52.359	2.942	21.592	19.484	-6.083
800	7.832	57.596	52.951	3.716	21.595	19.182	-5.240
900	7.988	58.528	53.520	4.507	21.600	18.880	-4.585
1000	8.123	59.377	54.064	5.313	21.605	18.577	-4.060
1100	8.238	60.157	54.583	6.131	21.610	18.274	-3.631
1200	8.336	60.878	55.078	6.960	21.615	17.971	-3.273
1300	8.419	61.548	55.550	7.798	21.619	17.668	-2.970
1400	8.491	62.175	56.001	8.644	21.623	17.364	-2.711
1500	8.552	62.763	56.432	9.496	21.625	17.059	-2.485
1600	8.605	63.317	56.846	10.354	21.626	16.754	-2.288
1700	8.651	63.840	57.242	11.217	21.627	16.450	-2.115
1800	8.692	64.335	57.622	12.084	21.626	16.147	-1.960
1900	8.727	64.806	57.988	12.955	21.624	15.842	-1.822
2000	8.759	65.255	58.340	13.829	21.619	15.536	-1.698

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.729 + 1.250\times10^{-3}T + 0.027\times10^{5}T^{-2}$

$H°- H°_{298} = 6.729\times10^{-3}T + 0.625\times10^{-6}T^{2} - 0.027\times10^{2}T^{-1} - 2.053$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 21.678 - 0.144\times10^{-3}T + 0.079\times10^{-6}T^{2} - 21.350T^{-1}$

$\Delta Gf° = 21.678 + 0.144\times10^{-3}T\ln T - 0.079\times10^{-6}T^{2} - 10.675T^{-1} - 4.000\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from JANAF (51).

$NO_2(g)$

Nitrogen Dioxide (ideal gas)

[Formation: $0.5N_2(g) + O_2(g) = NO_2(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.837	57.343	57.343	0	7.930	12.267	-8.992
300	8.850	57.398	57.345	.016	7.926	12.294	-8.956
400	9.601	60.046	57.699	.939	7.791	13.772	-7.525
500	10.327	62.268	58.396	1.936	7.706	15.279	-6.678
600	10.955	64.208	59.206	3.001	7.659	16.798	-6.119
700	11.469	65.937	60.047	4.123	7.640	18.323	-5.721
800	11.881	67.496	60.882	5.291	7.638	19.848	-5.422
900	12.208	68.915	61.697	6.496	7.649	21.374	-5.190
1000	12.468	70.215	62.485	7.730	7.669	22.898	-5.004
1100	12.677	71.414	63.243	8.988	7.694	24.420	-4.852
1200	12.847	72.524	63.970	10.265	7.723	25.941	-4.724
1300	12.985	73.558	64.669	11.556	7.753	27.457	-4.616
1400	13.099	74.525	65.339	12.861	7.783	28.971	-4.523
1500	13.193	75.432	65.981	14.176	7.813	30.484	-4.441
1600	13.273	76.286	66.599	15.499	7.841	31.994	-4.370
1700	13.340	77.093	67.193	16.830	7.869	33.502	-4.307
1800	13.398	77.857	67.764	18.167	7.894	35.011	-4.251
1900	13.447	78.583	68.315	19.509	7.916	36.515	-4.200
2000	13.490	79.274	68.846	20.856	7.935	38.020	-4.155

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.899 + 2.374x10^{-3}T - 1.573x10^{5}T^{-2}$

$H°- H°_{298} = 9.899x10^{-3}T + 1.187x10^{-6}T^{2} + 1.573x10^{2}T^{-1} - 3.584$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 7.682 - 0.590x10^{-3}T + 0.389x10^{-6}T^{2} + 116.050T^{-1}$

$\Delta Gf° = 7.682 + 0.590x10^{-3}T\ln T - 0.389x10^{-6}T^{2} + 58.025T^{-1} + 11.484x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from JANAF (51).

$N_2O(g)$

Dinitrogen Oxide (ideal gas)

[Formation: $N_2(g) + 0.5O_2(g) = N_2O(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.230	52.546	52.546	0	19.610	24.895	-18.248
300	9.250	52.603	52.546	.017	19.608	24.928	-18.160
400	10.201	55.400	52.920	.992	19.531	26.716	-14.597
500	10.953	57.761	53.659	2.051	19.521	28.514	-12.463
600	11.565	59.813	54.516	3.178	19.558	30.310	-11.040
700	12.070	61.635	55.406	4.360	19.624	32.097	-10.021
800	12.486	63.275	56.289	5.589	19.711	33.873	-9.254
900	12.830	64.766	57.149	6.855	19.811	35.637	-8.654
1000	13.113	66.133	57.980	8.153	19.920	37.390	-8.171
1100	13.348	67.394	58.779	9.476	20.036	39.132	-7.775
1200	13.544	68.565	59.548	10.821	20.157	40.861	-7.442
1300	13.707	69.655	60.283	12.184	20.281	42.584	-7.159
1400	13.845	70.676	60.989	13.562	20.406	44.294	-6.915
1500	13.961	71.635	61.667	14.952	20.531	45.996	-6.702
1600	14.060	72.540	62.319	16.353	20.658	47.688	-6.514
1700	14.145	73.395	62.946	17.764	20.785	49.374	-6.347
1800	14.218	74.205	63.548	19.182	20.911	51.054	-6.199
1900	14.282	74.976	64.130	20.607	21.036	52.723	-6.064
2000	14.337	75.710	64.691	22.038	21.160	54.388	-5.943

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.586 + 2.412\times10^{-3}T - 1.844\times10^{5}T^{-2}$

$H°- H°_{298} = 10.586\times10^{-3}T + 1.206\times10^{-6}T^{2} + 1.844\times10^{2}T^{-1} - 3.882$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 18.873 + 0.454\times10^{-3}T + 0.365\times10^{-6}T^{2} + 169.700T^{-1}$

$\Delta Gf° = 18.873 - 0.454\times10^{-3}T\ln T - 0.365\times10^{-6}T^{2} + 84.850T^{-1} + 21.940\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from JANAF (51).

$N_2O_3(g)$

Dinitrogen Trioxide (ideal gas)

[Formation: $N_2(g) + 1.5O_2(g) = N_2O_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	15.683	73.915	73.915	0	20.010	33.535	-24.581
300	15.718	74.012	73.915	.029	20.007	33.619	-24.491
400	17.385	78.771	74.554	1.687	19.903	38.175	-20.858
500	18.731	82.801	75.809	3.496	19.912	42.745	-18.684
600	19.821	86.316	77.274	5.425	19.996	47.304	-17.230
700	20.693	89.439	78.792	7.453	20.130	51.847	-16.187
800	21.386	92.249	80.301	9.558	20.295	56.366	-15.398
900	21.937	94.801	81.773	11.725	20.482	60.864	-14.780
1000	22.376	97.136	83.195	13.941	20.682	65.339	-14.280
1100	22.729	99.286	84.561	16.197	20.892	69.795	-13.867
1200	23.015	101.276	85.872	18.485	21.108	74.233	-13.519
1300	23.250	103.128	87.129	20.799	21.327	78.652	-13.222
1400	23.444	104.858	88.334	23.134	21.545	83.053	-12.965
1500	23.606	106.482	89.491	25.486	21.763	87.436	-12.739
1600	23.742	108.010	90.601	27.854	21.979	91.807	-12.540
1700	23.857	109.453	91.668	30.234	22.193	96.165	-12.363
1800	23.956	110.819	92.694	32.625	22.404	100.513	-12.204
1900	24.041	112.117	93.683	35.025	22.610	104.845	-12.060
2000	24.114	113.352	94.635	37.433	22.812	109.168	-11.929

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.419 + 3.758\times10^{-3}T - 3.429\times10^{5}T^{-2}$

$H°- H°_{298} = 18.419\times10^{-3}T + 1.879\times10^{-6}T^{2} + 3.429\times10^{2}T^{-1} - 6.809$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 18.698 + 1.057\times10^{-3}T + 0.536\times10^{-6}T^{2} + 283.000T^{-1}$

$\Delta Gf° = 18.698 - 1.057\times10^{-3}T\ln T - 0.536\times10^{-6}T^{2} + 141.500T^{-1} + 54.353\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from JANAF (51).

$N_2O_4(g)$

Dinitrogen Tetroxide (ideal gas)

[Formation: $N_2(g) + 2O_2(g) = N_2O_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.465	72.724	72.724	0	2.190	23.375	-17.134
300	18.520	72.838	72.725	.034	2.185	23.507	-17.125
400	21.157	78.542	73.484	2.023	2.057	30.639	-16.740
500	23.233	83.496	75.002	4.247	2.116	37.782	-16.514
600	24.860	87.881	76.789	6.655	2.301	44.900	-16.355
700	26.127	91.813	78.660	9.207	2.570	51.980	-16.229
800	27.113	95.369	80.530	11.871	2.895	59.014	-16.122
900	27.884	98.609	82.361	14.623	3.260	66.009	-16.029
1000	28.492	101.579	84.136	17.443	3.651	72.960	-15.945
1100	28.977	104.318	85.848	20.317	4.059	79.872	-15.869
1200	29.367	106.857	87.495	23.235	4.481	86.746	-15.798
1300	29.684	109.221	89.076	26.188	4.911	93.584	-15.733
1400	29.946	111.430	90.594	29.170	5.344	100.389	-15.671
1500	30.163	113.504	92.053	32.176	5.781	107.162	-15.613
1600	30.345	115.457	93.456	35.201	6.216	113.904	-15.558
1700	30.499	117.301	94.805	38.244	6.652	120.623	-15.507
1800	30.630	119.048	96.104	41.300	7.084	127.317	-15.458
1900	30.743	120.707	97.355	44.369	7.512	133.984	-15.411
2000	30.840	122.287	98.563	47.448	7.935	140.627	-15.367

Phase change: 294.25 K, boiling point of $N_2O_4(l)$ to equilibrium mixture of $N_2O_4(g)$ and $NO_2(g)$; ΔH° = 9.11 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 23.169 + 5.110\times10^{-3}T - 5.537\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 23.169\times10^{-3}T + 2.555\times10^{-6}T^2 + 5.537\times10^{2}T^{-1} - 8.992$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -0.129 + 2.192\times10^{-3}T + 0.960\times10^{-6}T^2 + 471.200T^{-1}$

$\Delta Gf^\circ = -0.129 - 2.192\times10^{-3}T\ln T - 0.960\times10^{-6}T^2 + 235.600T^{-1} + 88.960\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from JANAF (51).

$N_2O_5(g)$

Dinitrogen Pentoxide (ideal gas)

[Formation: $N_2(g) + 2.5O_2(g) = N_2O_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.017	82.801	82.801	0	2.700	28.186	-20.661
300	23.089	82.944	82.801	.043	2.697	28.345	-20.649
400	26.494	90.077	83.752	2.530	2.713	36.899	-20.160
500	28.965	96.270	85.648	5.311	2.963	45.422	-19.854
600	30.684	101.713	87.883	8.298	3.349	53.878	-19.625
700	31.891	106.539	90.209	11.431	3.810	62.265	-19.440
800	32.744	110.856	92.526	14.664	4.306	70.579	-19.281
900	33.365	114.750	94.782	17.971	4.819	78.834	-19.143
1000	33.806	118.289	96.958	21.331	5.336	87.030	-19.020
1100	34.137	121.527	99.047	24.728	5.848	95.175	-18.909
1200	34.410	124.509	101.046	28.156	6.356	103.275	-18.809
1300	34.612	127.271	102.958	31.607	6.855	111.332	-18.716
1400	34.782	129.842	104.787	35.077	7.344	119.349	-18.631
1500	34.913	132.246	106.538	38.562	7.826	127.333	-18.552
1600	35.027	134.503	108.216	42.060	8.295	135.285	-18.479
1700	35.105	136.629	109.825	45.566	8.753	143.208	-18.410
1800	35.177	138.638	111.371	49.080	9.199	151.106	-18.346
1900	35.242	140.542	112.857	52.601	9.632	158.975	-18.286
2000	35.302	142.351	114.286	56.129	10.055	166.825	-18.230

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 30.396 + 3.594\times10^{-3}T - 7.512\times10^{5}T^{-2}$

$H°- H°_{298} = 30.396\times10^{-3}T + 1.797\times10^{-6}T^{2} + 7.512\times10^{2}T^{-1} - 11.742$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -1.193 + 5.804\times10^{-3}T - 0.050\times10^{-6}T^{2} + 646.100T^{-1}$

$\Delta Gf° = -1.193 - 5.804\times10^{-3}T\ln T + 0.050\times10^{-6}T^{2} + 323.050T^{-1} + 127.959\times10^{-3}T$

Source: Data from JANAF (51).

Na(c,l,g)

Sodium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.730	12.298	12.298	0
300	6.741	12.340	12.300	.012
371	7.468	13.841	12.452	.515
371	7.596	15.517	12.452	1.137
400	7.531	16.086	12.696	1.356
500	7.302	17.741	13.547	2.097
600	7.124	19.056	14.359	2.818
700	6.996	20.143	15.109	3.524
800	6.918	21.072	15.798	4.219
900	6.892	21.885	16.431	4.909
1000	6.918	22.612	17.013	5.599
1100	6.993	23.274	17.551	6.295
1177	7.091	23.752	17.945	6.835
1177	4.968	43.535	17.945	30.120
1200	4.968	43.631	18.434	30.236
1300	4.968	44.030	20.390	30.732
1400	4.968	44.398	22.092	31.229
1500	4.968	44.740	23.589	31.726
1600	4.968	45.061	24.922	32.223
1700	4.969	45.362	26.115	32.720
1800	4.970	45.646	27.192	33.217
1900	4.971	45.915	28.171	33.714
2000	4.973	46.170	29.064	34.211
2100	4.975	46.413	29.885	34.708
2200	4.979	46.644	30.641	35.206
2300	4.985	46.866	31.343	35.704
2400	4.992	47.078	31.993	36.203
2500	5.001	47.282	32.601	36.703
2600	5.013	47.478	33.169	37.203
2700	5.027	47.668	33.703	37.705
2800	5.044	47.851	34.205	38.209
2900	5.065	48.028	34.678	38.714
3000	5.089	48.200	35.126	39.222

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1177 K, calculated boiling point to ideal monatomic gas; ΔH° = 23.285 kcal/mol.
1156 K, normal boiling point to equilibrium mixture of Na(g) and Na_2(g).

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-371 K: $Cp^\circ = 3.951 + 9.316\times10^{-3}T$

$H^\circ - H^\circ_{298} = 3.951\times10^{-3}T + 4.658\times10^{-6}T^2 - 1.592$

371-1177 K: $Cp^\circ = 7.004 - 0.184\times10^{-3}T + 0.909\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.004\times10^{-3}T - 0.092\times10^{-6}T^2 - 0.909\times10^{2}T^{-1} - 1.204$

1177-3000 K: $Cp^\circ = 4.967 + 0.008\times10^{-3}T - 0.110\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.967\times10^{-3}T + 0.004\times10^{-6}T^2 + 0.110\times10^{2}T^{-1} + 24.259$

Source: Data from JANAF (51).

Na(g)

Sodium (ideal monatomic gas)

[Formation: Na(c,l,g) = Na(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^{\circ}_{298})/T$	$H°-H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	4.968	36.714	36.714	0	25.755	18.475	-13.543
300	4.968	36.745	36.715	.009	25.752	18.431	-13.426
371	4.968	37.800	36.825	.362	25.602	16.713	-9.845
371	4.968	37.800	36.825	.362	24.980	16.713	-9.845
400	4.968	38.174	36.909	.506	24.905	16.070	-8.780
500	4.968	39.282	37.276	1.003	24.661	13.890	-6.071
600	4.968	40.188	37.688	1.500	24.437	11.758	-4.283
700	4.968	40.954	38.103	1.996	24.227	9.659	-3.016
800	4.968	41.617	38.501	2.493	24.029	7.593	-2.074
900	4.968	42.203	38.881	2.990	23.836	5.550	-1.348
1000	4.968	42.726	39.239	3.487	23.643	3.529	-.771
1100	4.968	43.200	39.578	3.984	23.444	1.525	-.303
1177	4.968	43.536	39.826	4.367	23.285	0	0
1177	4.968	43.536	39.826	4.367	0	0	0
1200	4.968	43.632	39.898	4.481	0	0	0
1300	4.968	44.030	40.202	4.977	0	0	0
1400	4.968	44.398	40.488	5.474	0	0	0
1500	4.968	44.740	40.759	5.971	0	0	0
1600	4.968	45.061	41.019	6.468	0	0	0
1700	4.969	45.362	41.265	6.965	0	0	0
1800	4.970	45.646	41.500	7.462	0	0	0
1900	4.971	45.915	41.726	7.959	0	0	0
2000	4.973	46.170	41.942	8.456	0	0	0
2100	4.975	46.413	42.150	8.953	0	0	0
2200	4.979	46.644	42.348	9.451	0	0	0
2300	4.985	46.866	42.540	9.949	0	0	0
2400	4.992	47.078	42.725	10.448	0	0	0
2500	5.001	47.282	42.903	10.948	0	0	0
2600	5.013	47.478	43.075	11.448	0	0	0
2700	5.027	47.668	43.242	11.950	0	0	0
2800	5.044	47.851	43.403	12.454	0	0	0
2900	5.065	48.028	43.559	12.959	0	0	0
3000	5.089	48.200	43.711	13.467	0	0	0

Phase changes: 371 K, melting point of Na; $\Delta H° = 0.622$ kcal/mol.
1177 K, boiling point of Na to ideal gas: $\Delta H° = 23.285$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 4.963 + 0.008\times10^{-3}T + 0.003\times10^{5}T^{-2}$

$H°-H^{\circ}_{298} = 4.963\times10^{-3}T + 0.004\times10^{-6}T^{2} - 0.003\times10^{2}T^{-1} - 1.479$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = 25.868 + 1.012\times10^{-3}T - 4.654\times10^{-6}T^{2} - 0.300T^{-1}$

$\Delta Gf° = 25.868 - 1.012\times10^{-3}T\ln T + 4.654\times10^{-6}T^{2} - 0.150T^{-1} - 20.415\times10^{-3}T$

371-1177 K: $\Delta Hf° = 25.480 - 2.041\times10^{-3}T + 0.096\times10^{-6}T^{2} + 90.600T^{-1}$

$\Delta Gf° = 25.480 + 2.041\times10^{-3}T\ln T - 0.096\times10^{-6}T^{2} + 45.300T^{-1} - 35.999\times10^{-3}T$

1177-3000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Source: Data from JANAF (51).

$Na_2(g)$

Sodium (ideal diatomic gas)

[Formation: $2Na(c,l,g) = Na_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.963	54.994	54.994	0	32.870	23.807	-17.451
300	8.965	55.050	54.994	.017	32.863	23.752	-17.303
371	9.020	56.960	55.195	.655	32.495	21.632	-12.743
371	9.020	56.960	55.195	.655	31.251	21.632	-12.743
400	9.043	57.640	55.347	.917	31.075	20.888	-11.412
500	9.101	59.665	56.015	1.825	30.501	18.409	-8.047
600	9.150	61.328	56.766	2.737	29.971	16.041	-5.843
700	9.195	62.742	57.522	3.654	29.476	13.757	-4.295
800	9.237	63.973	58.253	4.576	29.008	11.545	-3.154
900	9.279	65.063	58.950	5.502	28.554	9.390	-2.280
1000	9.319	66.043	59.611	6.432	28.104	7.285	-1.592
1100	9.359	66.933	60.237	7.366	27.646	5.223	-1.038
1177	9.390	67.567	60.696	8.087	27.287	3.673	-.682
1177	9.390	67.567	60.696	8.087	-19.283	3.673	-.682
1200	9.399	67.749	60.830	8.303	-19.299	4.117	-.750
1300	9.438	68.503	61.391	9.245	-19.349	6.075	-1.021
1400	9.477	69.204	61.925	10.191	-19.397	8.032	-1.254
1500	9.516	69.859	62.432	11.141	-19.441	9.991	-1.456
1600	9.555	70.474	62.915	12.094	-19.482	11.955	-1.633
1700	9.594	71.055	63.377	13.052	-19.518	13.919	-1.789
1800	9.633	71.604	63.819	14.013	-19.551	15.887	-1.929
1900	9.672	72.126	64.243	14.978	-19.580	17.858	-2.054
2000	9.711	72.623	64.649	15.948	-19.604	19.830	-2.167
2100	9.749	73.098	65.040	16.921	-19.625	21.804	-2.269
2200	9.788	73.552	65.417	17.897	-19.645	23.774	-2.362
2300	9.827	73.988	65.780	18.878	-19.660	25.751	-2.447
2400	9.865	74.407	66.131	19.863	-19.673	27.725	-2.525
2500	9.904	74.811	66.471	20.851	-19.685	29.698	-2.596
2600	9.942	75.200	66.798	21.844	-19.692	31.674	-2.662
2700	9.981	75.576	67.117	22.840	-19.700	33.652	-2.724
2800	10.020	75.940	67.426	23.840	-19.708	35.626	-2.781
2900	10.058	76.292	67.725	24.844	-19.714	37.602	-2.834
3000	10.097	76.634	68.017	25.851	-19.723	39.575	-2.883

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol of Na.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 8.941 + 0.386\times10^{-3}T - 0.083\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.941\times10^{-3}T + 0.193\times10^{-6}T^2 + 0.083\times10^{2}T^{-1} - 2.711$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = 33.343 + 1.039\times10^{-3}T - 9.123\times10^{-6}T^2 + 8.300T^{-1}$

$\Delta Gf^\circ = 33.343 - 1.039\times10^{-3}T\ln T + 9.123\times10^{-6}T^2 + 4.150T^{-1} - 28.833\times10^{-3}T$

371-1177 K: $\Delta Hf^\circ = 32.567 - 5.067\times10^{-3}T + 0.377\times10^{-6}T^2 + 190.100T^{-1}$

$\Delta Gf^\circ = 32.567 + 5.067\times10^{-3}T\ln T - 0.377\times10^{-6}T^2 + 95.050T^{-1} - 60.000\times10^{-3}T$

1177-3000 K: $\Delta Hf^\circ = -18.359 - 0.993\times10^{-3}T + 0.185\times10^{-6}T^2 - 13.700T^{-1}$

$\Delta Gf^\circ = -18.359 + 0.993\times10^{-3}T\ln T - 0.185\times10^{-6}T^2 - 6.850T^{-1} + 11.921\times10^{-3}T$

Source: Data from JANAF (51).

NaO(g)

Sodium Oxide (ideal gas)

[Formation: $Na(c,l,g) + 0.5O_2(g) = NaO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.400	54.737	54.737	0	20.000	14.652	-10.740
300	8.407	54.789	54.737	.016	19.998	14.620	-10.651
371	8.584	56.596	54.925	.620	19.848	13.362	-7.871
371	8.584	56.596	54.925	.620	19.226	13.362	-7.871
400	8.656	57.245	55.070	.870	19.153	12.907	-7.052
500	8.798	59.194	55.708	1.743	18.919	11.373	-4.971
600	8.888	60.806	56.426	2.628	18.705	9.885	-3.600
700	8.952	62.181	57.152	3.520	18.503	8.430	-2.632
800	9.002	63.380	57.858	4.418	18.307	7.004	-1.913
900	9.042	64.443	58.532	5.320	18.111	5.603	-1.361
1000	9.077	65.397	59.171	6.226	17.914	4.224	-.923
1100	9.108	66.264	59.778	7.135	17.708	2.863	-.569
1177	9.130	66.881	60.222	7.838	17.544	1.834	-.341
1177	9.130	66.881	60.222	7.838	-5.741	1.834	-.341
1200	9.137	67.058	60.351	8.048	-5.744	1.980	-.361
1300	9.163	67.790	60.895	8.963	-5.753	2.627	-.442
1400	9.188	68.470	61.413	9.880	-5.765	3.271	-.511
1500	9.213	69.105	61.905	10.800	-5.777	3.915	-.570
1600	9.236	69.700	62.373	11.723	-5.790	4.563	-.623
1700	9.259	70.261	62.822	12.647	-5.804	5.209	-.670
1800	9.281	70.791	63.249	13.575	-5.817	5.858	-.711
1900	9.304	71.293	63.659	14.504	-5.832	6.508	-.749
2000	9.325	71.771	64.054	15.435	-5.847	7.157	-.782

*All data except enthalpy of formation at 298 K estimated.

Phase changes: 371 K, melting point of Na; $\Delta H° = 0.622$ kcal/mol.
1177 K, boiling point of Na to ideal gas; $\Delta H° = 23.285$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.872 + 0.246\times10^{-3}T - 0.485\times10^{5}T^{-2}$

$H°- H°_{298} = 8.872\times10^{-3}T + 0.123\times10^{-6}T^{2} + 0.485\times10^{2}T^{-1} - 2.819$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = 19.949 + 1.306\times10^{-3}T - 4.786\times10^{-6}T^{2} + 25.900T^{-1}$

$\Delta Gf° = 19.949 - 1.306\times10^{-3}T\ln T + 4.786\times10^{-6}T^{2} + 12.950T^{-1} - 11.898\times10^{-3}T$

371-1177 K: $\Delta Hf° = 19.561 - 1.747\times10^{-3}T - 0.036\times10^{-6}T^{2} + 116.800T^{-1}$

$\Delta Gf° = 19.561 + 1.747\times10^{-3}T\ln T + 0.036\times10^{-6}T^{2} + 58.400T^{-1} - 27.482\times10^{-3}T$

1177-2000 K: $\Delta Hf° = -5.902 + 0.290\times10^{-3}T - 0.132\times10^{-6}T^{2} + 14.900T^{-1}$

$\Delta Gf° = -5.902 - 0.290\times10^{-3}T\ln T + 0.132\times10^{-6}T^{2} + 7.450T^{-1} + 8.479\times10^{-3}T$

Source: Data from JANAF (51) who estimated all except enthalpy of formation at 298 K.

$NaO_2(c)$

Sodium Dioxide, Sodium Superoxide

[Formation: $Na(c,1) + O_2(g) = NaO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.240	27.700	27.700	0	-62.300	-52.281	38.323
300*	17.241	27.807	27.700	.032	-62.293	-52.218	38.041
371	17.530	31.477	28.084	1.259	-62.071	-49.860	29.371
371	17.530	31.477	28.084	1.259	-62.693	-49.860	29.371
400	17.648	32.801	28.378	1.769	-62.610	-48.860	26.696
500	18.417	36.820	29.678	3.571	-62.280	-45.459	19.870
600	19.204	40.248	31.160	5.453	-61.874	-42.131	15.346
700	19.908	43.262	32.678	7.409	-61.402	-38.878	12.138
800	20.484	45.960	34.173	9.430	-60.874	-35.696	9.752
825	20.606	46.592	34.539	9.944	-60.735	-34.911	9.248

*Data above 298 K estimated.

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
825 K, melting point of NaO_2.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-825 K: $Cp^\circ = 13.412 + 9.024\times10^{-3}T + 1.012\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.412\times10^{-3}T + 4.512\times10^{-6}T^2 - 1.012\times10^{2}T^{-1} - 4.060$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -62.416 + 2.231\times10^{-3}T - 0.649\times10^{-6}T^2 - 146.400T^{-1}$

$\Delta Gf^\circ = -62.416 - 2.231\times10^{-3}T\ln T + 0.649\times10^{-6}T^2 - 73.200T^{-1} + 47.335\times10^{-3}T$

371-825 K: $\Delta Hf^\circ = -62.805 - 0.822\times10^{-3}T + 4.101\times10^{-6}T^2 - 55.500T^{-1}$

$\Delta Gf^\circ = -62.805 + 0.822\times10^{-3}T\ln T - 4.101\times10^{-6}T^2 - 27.750T^{-1} + 31.751\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from NBS (230). Low-temperature heat capacities and entropy at 298 K from Todd (221). High-temperature data estimated.

$Na_2O(c)$

Disodium Oxide

[Formation: $2Na(c,l,g) + 0.5O_2(g) = Na_2O(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	16.520	17.990	17.990	0	-99.700	-90.425	66.282
300	16.536	18.092	17.990	.031	-99.700	-90.366	65.831
371	17.278	21.683	18.364	1.232	-99.756	-88.153	51.929
371	17.278	21.683	18.364	1.232	-101.000	-88.153	51.929
400	17.581	22.995	18.653	1.737	-101.036	-87.148	47.615
500	18.518	27.022	19.934	3.544	-101.077	-83.667	36.570
600	19.228	30.465	21.410	5.433	-101.007	-80.190	29.209
700	19.768	33.471	22.922	7.384	-100.857	-76.733	23.957
800	20.319	36.145	24.411	9.387	-100.643	-73.300	20.024
900	21.162	38.582	25.852	11.457	-100.360	-69.898	16.973
1000	22.666	40.882	27.241	13.641	-99.970	-66.533	14.541
1100	25.290	43.155	28.584	16.028	-99.395	-63.218	12.560
1177	28.590	44.962	29.596	18.086	-98.742	-60.699	11.271
1177	28.590	44.962	29.596	18.086	-145.312	-60.699	11.271
1200	29.576	45.525	29.896	18.755	-144.974	-59.052	10.755
1300	36.152	48.134	31.196	22.019	-143.130	-51.957	8.735

Phase changes: 371 K, melting point of Na; $\Delta H° = 0.622$ kcal/mol.
1177 K, boiling point of Na to ideal gas; $\Delta H° = 23.285$ kcal/mol.
1405 K, melting point of Na_2O; $\Delta H° = 11.4 \pm .6$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp° = 13.377 + 9.834\times10^{-3}T + 0.187\times10^{5}T^{-2}$

$H°- H°_{298} = 13.377\times10^{-3}T + 4.917\times10^{-6}T^{2} - 0.187\times10^{2}T^{-1} - 4.363$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -99.703 + 1.860\times10^{-3}T - 4.650\times10^{-6}T^{2} - 41.300T^{-1}$

$\Delta Gf° = -99.703 - 1.860\times10^{-3}T\ln T + 4.650\times10^{-6}T^{2} - 20.650T^{-1} + 40.561\times10^{-3}T$

371-1177 K: $\Delta Hf° = -100.479 - 4.246\times10^{-3}T + 4.849\times10^{-6}T^{2} + 140.500T^{-1}$

$\Delta Gf° = -100.479 + 4.246\times10^{-3}T\ln T - 4.849\times10^{-6}T^{2} + 70.250T^{-1} + 9.393\times10^{-3}T$

1177-1300 K: $\Delta Hf° = -151.405 - 0.172\times10^{-3}T + 4.658\times10^{-6}T^{2} - 63.300T^{-1}$

$\Delta Gf° = -151.405 + 0.172\times10^{-3}T\ln T - 4.658\times10^{-6}T^{2} - 31.650T^{-1} + 81.314\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (239). Entropy at 298 K from Grimley (83). Other data based on Fredrickson (70).

$Na_2O_2(c)$

Disodium Dioxide, Sodium Peroxide

[Formation: $2Na(c,l) + O_2(g) = Na_2O_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	21.350	22.650	22.650	0	-122.300	-107.109	78.512
300	21.395	22.782	22.650	.040	-122.297	-107.013	77.958
371	22.757	27.485	23.135	1.614	-122.231	-103.404	60.913
371	22.757	27.485	23.135	1.614	-123.475	-103.404	60.913
400	23.314	29.219	23.514	2.282	-123.453	-101.836	55.640
500	24.722	34.578	25.206	4.686	-123.262	-96.450	42.158
600	25.929	39.195	27.162	7.220	-122.925	-91.117	33.189
700	27.040	43.276	29.177	9.869	-122.466	-85.852	26.804
785	27.943	46.425	30.877	12.205	-121.990	-81.433	22.671
785	27.080	48.145	30.877	13.555	-120.640	-81.433	22.671
800	27.080	48.657	31.206	13.961	-120.562	-80.684	22.042
900	27.080	51.847	33.326	16.669	-120.048	-75.730	18.390
948	27.080	53.254	34.299	17.969	-119.806	-73.373	16.915

Phase changes: 371 K, melting point of Na; $\Delta H°$ = 0.622 kcal/mol.
785 K, α - β transition point of Na_2O_2; $\Delta H°$ = 1.350 kcal/mol.
948 K, melting point of Na_2O_2; $\Delta H°$ unknown.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-785 K: $Cp° = 20.700 + 9.624\times10^{-3}T - 1.973\times10^{5}T^{-2}$

$H°- H°_{298} = 20.700\times10^{-3}T + 4.812\times10^{-6}T^2 + 1.973\times10^{2}T^{-1} - 7.261$

785-948 K: $Cp° = 27.080$

$H°- H°_{298} = 27.080\times10^{-3}T - 7.703$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -124.025 + 5.568\times10^{-3}T - 5.007\times10^{-6}T^2 + 152.100T^{-1}$

$\Delta Gf° = -124.025 - 5.568\times10^{-3}T\ln T + 5.007\times10^{-6}T^2 + 76.050T^{-1} + 86.113\times10^{-3}T$

371-785 K: $\Delta Hf° = -124.801 - 0.538\times10^{-3}T + 4.493\times10^{-6}T^2 + 333.900T^{-1}$

$\Delta Gf° = -124.801 + 0.538\times10^{-3}T\ln T - 4.493\times10^{-6}T^2 + 166.950T^{-1} + 54.945\times10^{-3}T$

785-948 K: $\Delta Hf° = -125.243 + 5.842\times10^{-3}T - 0.319\times10^{-6}T^2 + 136.600T^{-1}$

$\Delta Gf° = -125.243 - 5.842\times10^{-3}T\ln T + 0.319\times10^{-6}T^2 + 68.300T^{-1} + 94.418\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (239). Low-temperature heat capacities and entropy at 298 K from Todd (221). High-temperature data based on Chandrasekharaiah (28).

Nb(c,l)

Niobium

T, K	cal/mol•K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.880	8.700	8.700	0
300	5.880	8.740	8.703	.011
400	6.090	10.460	8.932	.611
500	6.180	11.830	9.378	1.226
600	6.280	12.970	9.888	1.849
700	6.380	13.940	10.394	2.482
800	6.480	14.800	10.892	3.126
900	6.580	15.570	11.372	3.778
1000	6.680	16.270	11.828	4.442
1100	6.780	16.910	12.259	5.116
1200	6.890	17.520	12.688	5.799
1300	7.020	18.080	13.085	6.493
1400	7.160	18.600	13.457	7.200
1500	7.310	19.100	13.818	7.923
1600	7.470	19.580	14.166	8.662
1700	7.630	20.040	14.501	9.417
1800	7.810	20.480	14.819	10.189
1900	8.000	20.900	15.122	10.979
2000	8.200	21.320	15.425	11.789
2100	8.410	21.720	15.711	12.619
2200	8.620	22.120	15.997	13.471
2300	8.850	22.510	16.273	14.344
2400	9.090	22.890	16.540	15.241
2500	9.330	23.270	16.805	16.162
2600	9.590	23.640	17.060	17.108
2700	9.860	24.000	17.304	18.080
2740	9.970	24.150	17.407	18.476
2740*	8.000	26.450	17.407	24.778
2800	8.000	26.620	17.599	25.258
2900	8.000	26.900	17.914	26.058
3000	8.000	27.180	18.227	26.858

*Enthalpy and entropy of fusion and data for Nb(l) estimated.

Phase change: 2740 K, melting point of Nb; ΔH° = 6.302 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2740 K: $Cp^\circ = 5.196 + 1.544\times10^{-3}T + 0.206\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.196\times10^{-3}T + 0.772\times10^{-6}T^2 - 0.206\times10^{2}T^{-1} - 1.549$

2740-3000 K: $Cp^\circ = 8.000$

$H^\circ - H^\circ_{298} = 8.000\times10^{-3}T + 2.858$

Sources: Data for Nb(s) based on Hultgren (99) and Berezin (16). Data for Nb(l) and enthalpy and entropy of fusion are those estimated by Hultgren (99).

Nb(g)

Niobium (ideal monatomic gas)

[Formation: Nb(c,1) = Nb(g)]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.208	44.490	44.490	0	175.200	164.529	-120.602
300	7.207	44.535	44.492	.013	175.202	164.463	-119.810
400	7.086	46.595	44.773	.729	175.318	160.864	-87.891
500	6.893	48.155	45.299	1.428	175.402	157.239	-68.728
600	6.704	49.395	45.882	2.108	175.459	153.604	-55.950
700	6.540	50.416	46.459	2.770	175.488	149.955	-46.817
800	6.402	51.280	47.009	3.417	175.491	146.307	-39.969
900	6.284	52.027	47.526	4.051	175.473	142.662	-34.643
1000	6.185	52.684	48.010	4.674	175.432	139.018	-30.382
1100	6.102	53.269	48.462	5.288	175.372	135.377	-26.897
1200	6.034	53.797	48.885	5.895	175.296	131.764	-23.997
1300	5.981	54.278	49.281	6.496	175.203	128.146	-21.543
1400	5.941	54.720	49.654	7.092	175.092	124.524	-19.439
1500	5.915	55.129	50.006	7.684	174.961	120.917	-17.617
1600	5.902	55.510	50.338	8.275	174.813	117.325	-16.026
1700	5.903	55.868	50.653	8.865	174.648	113.740	-14.622
1800	5.917	56.205	50.952	9.456	174.467	110.162	-13.375
1900	5.943	56.526	51.237	10.049	174.270	106.581	-12.259
2000	5.981	56.832	51.510	10.645	174.056	103.032	-11.259
2100	6.030	57.125	51.770	11.246	173.827	99.476	-10.353
2200	6.089	57.406	52.019	11.851	173.580	95.951	-9.532
2300	6.157	57.679	52.260	12.464	173.320	92.431	-8.783
2400	6.234	57.942	52.491	13.083	173.042	88.917	-8.097
2500	6.317	58.198	52.714	13.711	172.749	85.429	-7.468
2600	6.407	58.448	52.930	14.347	172.439	81.938	-6.887
2700	6.501	58.691	53.138	14.992	172.112	78.446	-6.350
2740	6.540	58.787	53.220	15.253	171.977	77.072	-6.147
2740	6.540	58.787	53.220	15.253	165.675	77.072	-6.147
2800	6.599	58.930	53.342	15.647	165.589	75.121	-5.863
2900	6.700	59.163	53.538	16.312	165.454	71.891	-5.418
3000	6.802	59.392	53.730	16.987	165.329	68.693	-5.004

Phase change: 2740 K, melting point of Nb ΔH° = 6.302 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 6.505 - 0.250\times10^{-3}T + 0.691\times10^{5}T^{-2}$

$H°- H°_{298} = 6.505\times10^{-3}T - 0.125\times10^{-6}T^{2} - 0.691\times10^{2}T^{-1} - 1.697$

Formation equations (kcal/mol):

298.15-2740 K: $\Delta Hf° = 175.052 + 1.309\times10^{-3}T - 0.897\times10^{-6}T^{2} - 48.500T^{-1}$

$\Delta Gf° = 175.052 - 1.309\times10^{-3}T\ln T + 0.897\times10^{-6}T^{2} - 24.250T^{-1} - 27.831\times10^{-3}T$

2740-3000 K: $\Delta Hf° = 170.645 - 1.495\times10^{-3}T - 0.125\times10^{-6}T^{2} - 69.100T^{-1}$

$\Delta Gf° = 170.645 + 1.495\times10^{-3}T\ln T + 0.125\times10^{-6}T^{2} - 34.550T^{-1} - 46.301\times10^{-3}T$

Source: Data from Chase (33).

NbO(c)

Niobium Oxide

[Formation: $Nb(c) + 0.5O_2(g) = NbO(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.860	11.500	11.500	0	-97.000	-90.529	66.359
300	9.875	11.561	11.501	.018	-97.000	-90.488	65.920
400	10.515	14.500	11.898	1.041	-96.932	-88.330	48.260
500	10.937	16.894	12.664	2.115	-96.838	-86.190	37.673
600	11.276	18.919	13.542	3.226	-96.728	-84.068	30.621
700	11.573	20.680	14.439	4.369	-96.606	-81.971	25.592
800	11.844	22.243	15.318	5.540	-96.479	-79.889	21.824
900	12.096	23.653	16.167	6.737	-96.340	-77.822	18.897
1000	12.335	24.940	16.981	7.959	-96.196	-75.771	16.560
1100	12.562	26.126	17.759	9.204	-96.044	-73.738	14.650
1200	12.779	27.229	18.503	10.471	-95.884	-71.698	13.058
1300	12.987	28.260	19.215	11.759	-95.718	-69.684	11.715
1400	13.186	29.230	19.896	13.068	-95.549	-67.693	10.567
1500	13.376	30.146	20.549	14.396	-95.379	-65.708	9.573
1600	13.559	31.015	21.176	15.743	-95.209	-63.730	8.705
1700	13.734	31.842	21.778	17.108	-95.040	-61.762	7.940
1800	13.901	32.632	22.360	18.489	-94.875	-59.813	7.262
1900	14.061	33.388	22.921	19.888	-94.713	-57.882	6.658
2000	14.214	34.113	23.462	21.301	-94.560	-55.939	6.113

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.287 + 2.096\times10^{-3}T - 0.935\times10^{5}T^{-2}$

$H°- H°_{298} = 10.287\times10^{-3}T + 1.048\times10^{-6}T^{2} + 0.935\times10^{2}T^{-1} - 3.474$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -97.749 + 1.476\times10^{-3}T + 0.024\times10^{-6}T^{2} + 91.500T^{-1}$

$\Delta Gf° = -97.749 - 1.476\times10^{-3}T\ln T - 0.024\times10^{-6}T^{2} + 45.750T^{-1} + 32.117\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (238). High-temperature data based on Gel'd (74).

NbO(g)

Niobium Oxide (ideal gas)

[Formation: $Nb(c,l) + 0.5O_2(g) = NbO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.358	57.090	57.090	0	47.500	40.378	-29.597
300	7.365	57.135	57.090	.014	47.496	40.335	-29.384
400	7.735	59.306	57.383	.769	47.297	37.976	-20.749
500	8.034	61.065	57.949	1.558	47.105	35.668	-15.590
600	8.253	62.550	58.595	2.373	46.920	33.401	-12.166
700	8.412	63.835	59.254	3.207	46.732	31.159	-9.728
800	8.529	64.967	59.900	4.054	46.535	28.946	-7.908
900	8.617	65.976	60.518	4.912	46.334	26.763	-6.499
1000	8.684	66.888	61.111	5.777	46.122	24.599	-5.376
1100	8.737	67.718	61.674	6.648	45.899	22.455	-4.461
1200	8.780	68.480	62.210	7.524	45.669	20.353	-3.707
1300	8.815	69.185	62.720	8.404	45.426	18.258	-3.069
1400	8.844	69.839	63.205	9.287	45.170	16.173	-2.525
1500	8.868	70.450	63.669	10.172	44.898	14.112	-2.056
1600	8.890	71.023	64.111	11.060	44.608	12.074	-1.649
1700	8.909	71.563	64.534	11.950	44.302	10.054	-1.292
1800	8.927	72.072	64.938	12.842	43.978	8.048	-.977
1900	8.944	72.555	65.326	13.736	43.635	6.048	-.696
2000	8.961	73.015	65.700	14.631	43.271	4.087	-.447
2100	8.978	73.452	66.058	15.528	42.885	2.128	-.221
2200	8.996	73.870	66.404	16.426	42.476	.204	-.020
2300	9.014	74.271	66.738	17.327	42.046	-1.705	.162
2400	9.035	74.655	67.060	18.229	41.591	-3.601	.328
2500	9.057	75.024	67.370	19.134	41.112	-5.463	.478
2600	9.081	75.380	67.672	20.041	40.607	-7.320	.615
2700	9.108	75.723	67.964	20.950	40.076	-9.172	.742
2740	9.120	75.857	68.078	21.315	39.857	-9.888	.789
2740	9.120	75.857	68.078	21.315	33.555	-9.888	.789
2800	9.137	76.055	68.247	21.862	33.340	-10.846	.847
2900	9.169	76.376	68.522	22.778	32.982	-12.418	.936
3000	9.203	76.687	68.788	23.696	32.625	-13.951	1.016

Phase change: 2740 K, melting point of Nb; $\Delta H° = 6.302$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 8.389 + 0.310\times10^{-3}T - 0.999\times10^{5}T^{-2}$

$H°- H°_{298} = 8.389\times10^{-3}T + 0.155\times10^{-6}T^{2} + 0.999\times10^{2}T^{-1} - 2.850$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 47.375 - 0.422\times10^{-3}T - 0.868\times10^{-6}T^{2} + 97.900T^{-1}$

$\Delta Gf° = 47.375 + 0.422\times10^{-3}T\ln T + 0.868\times10^{-6}T^{2} + 48.950T^{-1} - 26.681\times10^{-3}T$

2000-2740 K: $\Delta Hf° = 48.043 - 0.977\times10^{-3}T - 0.722\times10^{-6}T^{2} - 194.500T^{-1}$

$\Delta Gf° = 48.043 + 0.977\times10^{-3}T\ln T + 0.722\times10^{-6}T^{2} - 97.250T^{-1} - 30.903\times10^{-3}T$

2740-3000 K: $\Delta Hf° = 43.635 - 3.781\times10^{-3}T + 0.050\times10^{-6}T^{2} - 215.100T^{-1}$

$\Delta Gf° = 43.635 + 3.781\times10^{-3}T\ln T - 0.050\times10^{-6}T^{2} - 107.550T^{-1} - 49.374\times10^{-3}T$

Source: Data from Chase (33).

NbO_2(c)

Niobium Dioxide

[Formation: Nb(c) + O_2(g) = NbO_2(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.740	13.030	13.030	0	-190.300	-176.980	129.728
300	13.772	13.115	13.032	.025	-190.299	-176.897	128.868
400	15.172	17.279	13.589	1.476	-190.158	-172.450	94.221
500	16.420	20.809	14.689	3.060	-189.920	-168.049	73.453
600	17.041	23.864	15.969	4.737	-189.621	-163.699	59.627
700	17.741	26.537	17.291	6.472	-189.297	-159.408	49.769
800	19.033	28.985	18.603	8.306	-188.905	-155.165	42.389
900	20.644	31.317	19.886	10.288	-188.389	-150.974	36.661
1000	23.990	33.629	21.144	12.485	-187.683	-146.852	32.094
1090	35.740	36.087	22.270	15.060	-186.469	-143.224	28.717
1090	22.000	36.087	22.270	15.060	-186.469	-143.224	28.717
1100	22.000	36.288	22.397	15.280	-186.401	-142.828	28.377
1200	22.000	38.203	23.636	17.480	-185.732	-138.878	25.293
1200	19.900	38.203	23.636	17.480	-185.732	-138.878	25.293
1300	19.900	39.796	24.819	19.470	-185.292	-134.986	22.693
1400	19.900	41.270	25.941	21.460	-184.873	-131.137	20.471
1500	19.900	42.643	27.010	23.450	-184.476	-127.311	18.549
1600	19.900	43.928	28.028	25.440	-184.102	-123.508	16.870
1700	19.900	45.134	28.999	27.430	-183.749	-119.727	15.392
1800	19.900	46.271	29.927	29.420	-183.419	-115.971	14.081
1900	19.900	47.347	30.815	31.410	-183.113	-112.247	12.911
2000	19.900	48.368	31.668	33.400	-182.832	-108.516	11.858

Phase changes: 1090 K, second order transition point of NbO_2; $\Delta H° = 0$ kcal/mol.
1200 K, second order transition point of NbO_2; $\Delta H° = 0$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1090 K: $Cp° = 7.405 + 16.132\times10^{-3}T + 1.356\times10^{5}T^{-2}$

$H°- H°_{298} = 7.405\times10^{-3}T + 8.066\times10^{-6}T^2 - 1.356\times10^{2}T^{-1} - 2.470$

1090-1200 K: $Cp° = 22.000$

$H°- H°_{298} = 22.000\times10^{-3}T - 8.920$

1200-2000 K: $Cp° = 19.900$

$H°- H°_{298} = 19.900\times10^{-3}T - 6.400$

Formation equations (kcal/mol):

298.15-1090 K: $\Delta Hf° = -188.869 - 5.021\times10^{-3}T + 6.791\times10^{-6}T^2 - 160.200T^{-1}$

$\Delta Gf° = -188.869 + 5.021\times10^{-3}T\ln T - 6.791\times10^{-6}T^2 - 80.100T^{-1} + 14.195\times10^{-3}T$

1090-1200 K: $\Delta Hf° = -195.319 + 9.574\times10^{-3}T - 1.275\times10^{-6}T^2 - 24.600T^{-1}$

$\Delta Gf° = -195.319 - 9.574\times10^{-3}T\ln T + 1.275\times10^{-6}T^2 - 12.300T^{-1} + 113.339\times10^{-3}T$

1200-2000 K: $\Delta Hf° = -192.799 + 7.474\times10^{-3}T - 1.275\times10^{-6}T^2 - 24.600T^{-1}$

$\Delta Gf° = -192.799 - 7.474\times10^{-3}T\ln T + 1.275\times10^{-6}T^2 - 12.300T^{-1} + 96.350\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (238). Low-temperature heat capacities and entropy at 298 from King (128). High-temperature data based on King (130).

$NbO_2(g)$

Niobium Dioxide (ideal gas)

[Formation: $Nb(c,l) + O_2(g) = NbO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15*	10.494	65.019	65.019	0	-47.800	-49.981	36.636
300	10.512	65.084	65.021	.019	-47.805	-49.993	36.420
400	11.382	68.233	65.443	1.116	-48.018	-50.691	27.696
500	12.025	70.846	66.270	2.288	-48.192	-51.340	22.440
600	12.476	73.080	67.223	3.514	-48.344	-51.952	18.923
700	12.794	75.029	68.202	4.779	-48.490	-52.545	16.405
800	13.022	76.753	69.165	6.070	-48.641	-53.115	14.510
900	13.189	78.297	70.096	7.381	-48.796	-53.663	13.031
1000	13.314	79.693	70.986	8.707	-48.961	-54.194	11.844
1100	13.411	80.967	71.837	10.043	-49.138	-54.712	10.870
1200	13.486	82.137	72.647	11.388	-49.324	-55.191	10.051
1300	13.545	83.219	73.419	12.740	-49.522	-55.666	9.358
1400	13.593	84.225	74.156	14.097	-49.736	-56.137	8.763
1500	13.632	85.164	74.859	15.458	-49.968	-56.585	8.244
1600	13.665	86.045	75.531	16.823	-50.219	-57.013	7.787
1700	13.692	86.874	76.173	18.191	-50.488	-57.424	7.382
1800	13.715	87.657	76.790	19.561	-50.778	-57.825	7.021
1900	13.735	88.399	77.381	20.934	-51.089	-58.222	6.697
2000	13.751	89.104	77.950	22.308	-51.424	-58.580	6.401
2100	13.766	89.776	78.498	23.684	-51.783	-58.940	6.134
2200	13.778	90.416	79.025	25.061	-52.168	-59.263	5.887
2300	13.789	91.029	79.533	26.440	-52.578	-59.572	5.661
2400	13.799	91.616	80.025	27.819	-53.017	-59.871	5.452
2500	13.808	92.180	80.500	29.199	-53.484	-60.139	5.257
2600	13.815	92.721	80.959	30.581	-53.979	-60.396	5.077
2700	13.822	93.243	81.405	31.962	-54.506	-60.654	4.910
2740	13.824	93.446	81.580	32.515	-54.725	-60.731	4.844
2740	13.824	93.446	81.580	32.515	-61.027	-60.731	4.844
2800	13.828	93.746	81.837	33.345	-61.242	-60.730	4.740
2900	13.834	94.231	82.256	34.728	-61.605	-60.706	4.575
3000	13.839	94.700	82.663	36.112	-61.972	-60.643	4.418

*All data except enthalpy of formation at 298 K estimated.

Phase change: 2740 K, melting point of Nb" $\Delta H°$ = 6.302 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 12.914 + 0.466\times10^{-3}T - 2.275\times10^{5}T^{-2}$

$H°- H°_{298} = 12.914\times10^{-3}T + 0.233\times10^{-6}T^2 + 2.275\times10^{2}T^{-1} - 4.634$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -48.533 + 0.488\times10^{-3}T - 1.042\times10^{-6}T^2 + 202.900T^{-1}$

$\Delta Gf° = -48.533 - 0.488\times10^{-3}T\ln T + 1.042\times10^{-6}T^2 + 101.450T^{-1} - 3.526\times10^{-3}T$

2000-2740 K: $\Delta Hf° = -47.197 - 0.622\times10^{-3}T - 0.748\times10^{-6}T^2 - 381.900T^{-1}$

$\Delta Gf° = -47.197 + 0.622\times10^{-3}T\ln T + 0.748\times10^{-6}T^2 - 190.950T^{-1} - 11.970\times10^{-3}T$

2740-3000 K: $\Delta Hf° = -51.604 - 3.426\times10^{-3}T + 0.024\times10^{-6}T^2 - 402.500T^{-1}$

$\Delta Gf° = -51.604 + 3.426\times10^{-3}T\ln T - 0.024\times10^{-6}T^2 - 201.250T^{-1} - 30.440\times10^{-3}T$

Source: Data from Chase (33) who estimated all except enthalpy of formation at 298 K.

$Nb_2O_5(c,1)$

Diniobium Pentoxide

[Formation: $2Nb(c) + 2.5O_2(g) = Nb_2O_5(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	31.570	32.800	32.800	0	-454.000	-422.064	309.378
300	31.655	32.996	32.803	.058	-453.996	-421.865	307.324
400	34.742	42.586	34.088	3.399	-453.631	-411.207	224.670
500	36.718	50.559	36.607	6.976	-453.111	-400.659	175.126
600	38.306	57.400	39.517	10.730	-452.490	-390.221	142.136
700	39.552	63.402	42.508	14.626	-451.805	-379.903	118.610
800	40.487	68.748	45.461	18.630	-451.085	-369.683	100.991
900	41.172	73.558	48.319	22.715	-450.339	-359.547	87.309
1000	41.684	77.924	51.065	26.859	-449.590	-349.499	76.382
1100	42.098	81.917	53.691	31.049	-448.845	-339.530	67.457
1200	42.488	85.597	56.199	35.278	-448.103	-329.587	60.025
1300	42.911	89.014	58.593	39.547	-447.362	-319.729	53.751
1400	43.412	92.212	60.881	43.863	-446.620	-309.951	48.385
1500	44.019	95.227	63.072	48.233	-445.871	-300.212	43.740
1600	44.740	98.090	65.171	52.670	-445.104	-290.516	39.682
1700	45.566	100.827	67.189	57.185	-444.304	-280.869	36.108
1785	46.330	103.068	68.844	61.090	-443.595	-272.717	33.390
1785	58.000	116.844	68.844	85.680	-419.005	-272.717	33.390
1800	58.000	117.329	69.246	86.550	-418.703	-271.488	32.963
1900	58.000	120.465	71.860	92.350	-416.718	-263.393	30.297
2000	58.000	123.440	74.365	98.150	-414.785	-255.355	27.904

Phase change: 1785 K, melting point of Nb_2O_5; $\Delta H° = 24.590$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1785 K: $Cp° = 36.773 + 5.226\times10^{-3}T - 6.010\times10^{5}T^{-2}$

$H°- H°_{298} = 36.773\times10^{-3}T + 2.613\times10^{-6}T^2 + 6.010\times10^{2}T^{-1} - 13.212$

1785-2000 K: $Cp° = 58.000$

$H°- H°_{298} = 58.000\times10^{-3}T - 17.850$

Formation equations (kcal/mol):

298.15-1785 K: $\Delta Hf° = -458.235 + 8.306\times10^{-3}T - 0.189\times10^{-6}T^2 + 529.200T^{-1}$

$\Delta Gf° = -458.235 - 8.306\times10^{-3}T\ln T + 0.189\times10^{-6}T^2 + 264.600T^{-1} + 165.607\times10^{-3}T$

1785-2000 K: $\Delta Hf° = -462.873 + 29.533\times10^{-3}T - 2.802\times10^{-6}T^2 - 71.800T^{-1}$

$\Delta Gf° = -462.873 - 29.533\times10^{-3}T\ln T + 2.802\times10^{-6}T^2 - 35.900T^{-1} + 322.566\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (238). Low-temperature heat capacities and entropy at 298 K from King (126). High-temperature data based on Orr (171).

Nd(c,l)

Neodymium

T, K	cal/mol•K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.550	17.100	17.100	0
300	6.560	17.140	17.103	.011
400	6.880	19.070	17.362	.683
500	7.240	20.640	17.862	1.389
600	7.660	22.000	18.443	2.134
700	8.140	23.220	19.044	2.923
800	8.710	24.340	19.634	3.765
900	9.340	25.400	20.214	4.667
1000	10.030	26.420	20.785	5.635
1100	10.780	27.410	21.342	6.675
1128	10.990	27.680	21.491	6.980
1128	10.660	28.320	21.491	7.704
1200	10.660	28.980	21.920	8.472
1289	10.660	29.740	22.430	9.420
1289	10.520	31.060	22.430	11.127
1300	10.520	31.150	22.502	11.243
1400	10.520	31.930	23.148	12.295
1500	10.520	32.650	23.752	13.347
1600	10.520	33.330	24.331	14.399
1700	10.520	33.970	24.881	15.451
1800	10.520	34.570	25.402	16.503
1900	10.520	35.140	25.901	17.555
2000	10.520	35.680	26.377	18.607

Phase changes: 1128 K, α - β transition point of Nd; ΔH° = 0.724 kcal/mol.
1289 K, melting point of Nd; ΔH° = 1.707 kcal/mol.
3341 K, boiling point of Nd; ΔH° = 65.3 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1128 K: $Cp^\circ = 3.968 + 5.930\times10^{-3}T + 0.724\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 3.968\times10^{-3}T + 2.965\times10^{-6}T^2 - 0.724\times10^{2}T^{-1} - 1.204$

1128-1289 K: $Cp^\circ = 10.658$

$H^\circ - H^\circ_{298} = 10.658\times10^{-3}T - 4.318$

1289-2000 K: $Cp^\circ = 10.520$

$H^\circ - H^\circ_{298} = 10.520\times10^{-3}T - 2.433$

Sources: Entropy at 298 K from Schumm (192). Data for Nd(c) from Hultgren (99). Data for Nd(l) based on Stretz (212).

Nd(g)

Neodymium (ideal monatomic gas)

[Formation: Nd(c,l) = Nd(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.280	45.243	45.243	0	78.300	69.909	-51.244
300	5.287	45.276	45.243	.010	78.299	69.858	-50.891
400	5.672	46.849	45.454	.558	78.175	67.063	-36.641
500	6.017	48.153	45.867	1.143	78.054	64.298	-28.104
600	6.285	49.275	46.345	1.758	77.924	61.559	-22.423
700	6.487	50.260	46.834	2.398	77.775	58.847	-18.373
800	6.643	51.137	47.319	3.054	77.589	56.151	-15.340
900	6.766	51.926	47.787	3.725	77.358	53.485	-12.988
1000	6.868	52.645	48.238	4.407	77.072	50.847	-11.112
1100	6.955	53.303	48.668	5.098	76.723	48.241	-9.584
1128	6.977	53.478	48.786	5.293	76.613	47.512	-9.205
1128	6.977	53.478	48.786	5.293	75.889	47.512	-9.205
1200	7.033	53.912	49.080	5.798	75.626	45.708	-8.324
1289	7.095	54.418	49.432	6.426	75.306	43.494	-7.374
1289	7.095	54.418	49.432	6.426	73.599	43.494	-7.374
1300	7.103	54.478	49.475	6.504	73.561	43.235	-7.268
1400	7.168	55.006	49.850	7.218	73.223	40.917	-6.387
1500	7.230	55.503	50.211	7.938	72.891	38.612	-5.626
1600	7.287	55.972	50.557	8.664	72.565	36.338	-4.963
1700	7.341	56.415	50.889	9.395	72.244	34.088	-4.382
1800	7.391	56.836	51.207	10.132	71.929	31.850	-3.867
1900	7.437	57.237	51.514	10.873	71.618	29.634	-3.409
2000	7.480	57.619	51.809	11.619	71.312	27.434	-2.998

Phase changes: 1128 K, α - β transition point of Nd; $\Delta H° = 0.724$ kcal/mol.
1289 K, melting point of Nd; $\Delta H° = 1.707$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 5.998 + 0.858\times10^{-3}T - 0.866\times10^{5}T^{-2}$

$H°- H°_{298} = 5.998\times10^{-3}T + 0.429\times10^{-6}T^{2} + 0.866\times10^{2}T^{-1} - 2.117$

Formation equations (kcal/mol):

298.15-1128 K: $\Delta Hf° = 77.387 + 2.030\times10^{-3}T - 2.536\times10^{-6}T^{2} + 159.000T^{-1}$

$\Delta Gf° = 77.387 - 2.030\times10^{-3}T\ln T + 2.536\times10^{-6}T^{2} + 79.500T^{-1} - 15.165\times10^{-3}T$

1128-1289 K: $\Delta Hf° = 80.501 - 4.660\times10^{-3}T + 0.429\times10^{-6}T^{2} + 86.600T^{-1}$

$\Delta Gf° = 80.501 + 4.660\times10^{-3}T\ln T - 0.429\times10^{-6}T^{2} + 43.300T^{-1} - 61.571\times10^{-3}T$

1289-2000 K: $\Delta Hf° = 78.616 - 4.522\times10^{-3}T + 0.429\times10^{-6}T^{2} + 86.600T^{-1}$

$\Delta Gf° = 78.616 + 4.522\times10^{-3}T\ln T - 0.429\times10^{-6}T^{2} + 43.300T^{-1} - 59.120\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). All other data from Feber (58).

Nd_2O_3(c)

Dineodymium Trioxide, Neodymium Sesquioxide

[Formation: $2Nd(c,l) + 1.5O_2(g) = Nd_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	26.610	37.900	37.900	0	-432.100	-411.287	301.478
300	26.662	38.065	37.902	.049	-432.092	-411.156	299.523
400	28.717	46.058	38.978	2.832	-431.719	-404.232	220.859
500	29.992	52.609	41.067	5.771	-431.288	-397.412	173.706
600	31.068	58.174	43.467	8.824	-430.858	-390.675	142.301
700	32.063	63.038	45.921	11.982	-430.445	-384.002	119.889
800	32.995	67.382	48.338	15.235	-430.073	-377.402	103.100
900	33.853	71.318	50.676	18.578	-429.755	-370.840	90.051
1000	34.632	74.926	52.923	22.003	-429.506	-364.307	79.618
1100	35.336	78.260	55.076	25.502	-429.345	-357.796	71.087
1128	35.519	79.150	55.663	26.494	-429.318	-355.986	68.971
1128	35.519	79.150	55.663	26.494	-430.766	-355.986	68.971
1200	35.988	81.363	57.140	29.068	-430.646	-351.219	63.965
1289	36.561	83.958	58.903	32.296	-430.455	-345.345	58.553
1289	36.561	83.958	58.903	32.296	-433.869	-345.345	58.553
1300	36.632	84.269	59.116	32.699	-433.841	-344.595	57.931
1395	37.294	86.875	60.918	36.210	-433.559	-338.082	52.965
1395	37.200	86.975	60.918	36.350	-433.419	-338.081	52.965
1400	37.200	87.109	61.012	36.536	-433.404	-337.741	52.723
1500	37.200	89.675	62.838	40.256	-433.092	-330.936	48.217
1600	37.200	92.076	64.591	43.976	-432.792	-324.132	44.274
1700	37.200	94.331	66.275	47.696	-432.499	-317.341	40.796
1800	37.200	96.457	67.893	51.416	-432.215	-310.578	37.709
1900	37.200	98.469	69.450	55.136	-431.940	-303.826	34.947
2000	37.200	100.377	70.949	58.856	-431.673	-297.089	32.464

Phase changes: 1128 K, α - β transition point of Nd; $\Delta H°$ = 0.724 kcal/mol.
1289 K, melting point of Nd; $\Delta H°$ = 1.707 kcal/mol.
1395 K, α - β transition point of Nd_2O_3; $\Delta H°$ = 0.140 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1395 K: $Cp° = 27.611 + 7.174\times10^{-3}T - 2.792\times10^{5}T^{-2}$

$H°- H°_{298} = 27.611\times10^{-3}T + 3.587\times10^{-6}T^{2} + 2.792\times10^{2}T^{-1} - 9.488$

1395-2000 K: $Cp° = 37.200$

$H°- H°_{298} = 37.200\times10^{-3}T - 15.544$

Formation equations (kcal/mol):

298.15-1128 K: $\Delta Hf° = -435.652 + 8.830\times10^{-3}T - 3.098\times10^{-6}T^{2} + 356.200T^{-1}$

$\Delta Gf° = -435.652 - 8.830\times10^{-3}T\ln T + 3.098\times10^{-6}T^{2} + 178.100T^{-1} + 129.104\times10^{-3}T$

1128-1289 K: $\Delta Hf° = -429.424 - 4.550\times10^{-3}T + 2.832\times10^{-6}T^{2} + 211.400T^{-1}$

$\Delta Gf° = -429.424 + 4.550\times10^{-3}T\ln T - 2.832\times10^{-6}T^{2} + 105.700T^{-1} + 36.291\times10^{-3}T$

1289-1395 K: $\Delta Hf° = -433.194 - 4.274\times10^{-3}T + 2.832\times10^{-6}T^{2} + 211.400T^{-1}$

$\Delta Gf° = -433.194 + 4.274\times10^{-3}T\ln T - 2.832\times10^{-6}T^{2} + 105.700T^{-1} + 41.192\times10^{-3}T$

1395-2000 K: $\Delta Hf° = -439.250 + 5.315\times10^{-3}T - 0.754\times10^{-6}T^{2} - 67.800T^{-1}$

$\Delta Gf° = -439.250 - 5.315\times10^{-3}T\ln T + 0.754\times10^{-6}T^{2} - 33.900T^{-1} + 110.032\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). Low-temperature heat capacities and entropy at 298 K from Justice (109). High-temperature data based on Pankratz (179) and Blomeke (19).

Ne(g)

Neon

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	4.968	34.947	34.947	0
300	4.968	34.978	34.948	.009
400	4.968	36.407	35.142	.506
500	4.968	37.515	35.509	1.003
600	4.968	38.421	35.921	1.500
700	4.968	39.187	36.336	1.996
800	4.968	39.850	36.734	2.493
900	4.968	40.436	37.114	2.990
1000	4.968	40.959	37.472	3.487
1100	4.968	41.433	37.811	3.984
1200	4.968	41.865	38.132	4.480
1300	4.968	42.262	38.434	4.977
1400	4.968	42.631	38.721	5.474
1500	4.968	42.973	38.992	5.971
1600	4.968	43.294	39.251	6.468
1700	4.968	43.595	39.499	6.964
1800	4.968	43.879	39.734	7.461
1900	4.968	44.148	39.960	7.958
2000	4.968	44.403	40.175	8.455
2100	4.968	44.645	40.382	8.952
2200	4.968	44.876	40.581	9.448
2300	4.968	45.097	40.773	9.945
2400	4.968	45.308	40.957	10.442
2500	4.968	45.511	41.135	10.939
2600	4.968	45.706	41.308	11.436
2700	4.968	45.893	41.474	11.932
2800	4.968	46.074	41.635	12.429
2900	4.968	46.248	41.791	12.926
3000	4.968	46.417	41.943	13.423

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $C_p^\circ = 4.968$

$H^\circ - H^\circ_{298} = 4.968 \times 10^{-3} T - 1.481$

Source: Data from JANAF (52).

Ni(c,1)

Nickel

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.210	7.140	7.140	0
300	6.220	7.180	7.140	.012
400	6.810	9.050	7.390	.664
500	7.420	10.630	7.882	1.374
600	8.330	12.050	8.457	2.156
631	9.520	12.490	8.647	2.425
700	7.360	13.290	9.070	2.954
800	7.410	14.270	9.656	3.691
900	7.550	15.150	10.218	4.439
1000	7.700	15.950	10.749	5.201
1100	7.870	16.700	11.265	5.979
1200	8.050	17.390	11.744	6.775
1300	8.250	18.040	12.202	7.590
1400	8.460	18.660	12.642	8.425
1500	8.680	19.250	13.062	9.282
1600	8.910	19.820	13.469	10.162
1700	9.150	20.360	13.852	11.064
1728	9.210	20.520	13.967	11.321
1728	9.300	22.890	13.967	15.421
1800	9.300	23.270	14.331	16.091
1900	9.300	23.770	14.812	17.021
2000	9.300	24.250	15.274	17.951

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.
3187 K, boiling point of Ni; ΔH° = 88.5 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-631 K: $Cp^\circ = 2.996 + 8.560\times10^{-3}T + 0.590\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 2.996\times10^{-3}T + 4.280\times10^{-6}T^2 - 0.590\times10^{2}T^{-1} - 1.076$

631-750 K: $Cp^\circ = 11.320 - 5.490\times10^{-3}T$

$H^\circ - H^\circ_{298} = 11.320\times10^{-3}T - 2.745\times10^{-6}T^2 - 3.625$

750-1728 K: $Cp^\circ = 5.071 + 2.314\times10^{-3}T + 3.136\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.071\times10^{-3}T + 1.157\times10^{-6}T^2 - 3.136\times10^{2}T^{-1} - 0.714$

1728-2000 K: $Cp^\circ = 9.300$

$H^\circ - H^\circ_{298} = 9.300\times10^{-3}T - 0.649$

Sources: Boiling point data from Hultgren (99). All other data from Mah (150).

Ni(g)

Nickel (ideal monatomic gas)

[Formation: Ni(c,l) = Ni(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.583	43.519	43.519	0	102.800	91.954	-67.403
300	5.585	43.553	43.520	.010	102.798	91.886	-66.938
400	5.702	45.175	43.740	.574	102.710	88.260	-48.222
500	5.825	46.461	44.159	1.151	102.577	84.662	-37.005
600	5.912	47.531	44.634	1.738	102.382	81.093	-29.538
631	5.926	47.829	44.784	1.921	102.296	79.997	-27.707
700	5.957	48.446	45.115	2.332	102.178	77.569	-24.218
800	5.971	49.243	45.583	2.928	102.037	74.059	-20.232
900	5.961	49.946	46.029	3.525	101.886	70.570	-17.136
1000	5.937	50.573	46.453	4.120	101.719	67.096	-14.664
1100	5.904	51.137	46.853	4.712	101.533	63.652	-12.646
1200	5.865	51.649	47.231	5.301	101.326	60.215	-10.967
1300	5.823	52.117	47.590	5.885	101.095	56.795	-9.548
1400	5.781	52.547	47.929	6.465	100.840	53.398	-8.336
1500	5.739	52.944	48.250	7.041	100.559	50.018	-7.288
1600	5.698	53.313	48.555	7.613	100.251	46.662	-6.374
1700	5.659	53.658	48.846	8.181	99.917	43.310	-5.568
1728	5.649	53.750	48.924	8.339	99.818	42.394	-5.362
1728	5.649	53.750	48.924	8.339	95.718	42.394	-5.362
1800	5.622	53.980	49.122	8.745	95.454	40.176	-4.878
1900	5.588	54.283	49.385	9.306	95.085	37.110	-4.269
2000	5.556	54.569	49.638	9.863	94.712	34.074	-3.723

Phase changes: 631 K, Curie temperature of Ni; $\Delta H° = 0$ kcal/mol.
1728 K, melting point of Ni; $\Delta H° = 4.100$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.196 - 0.272\times10^{-3}T - 0.473\times10^{5}T^{-2}$

$H°- H°_{298} = 6.196\times10^{-3}T - 0.136\times10^{-6}T^{2} + 0.473\times10^{2}T^{-1} - 1.994$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf° = 101.882 + 3.200\times10^{-3}T - 4.416\times10^{-6}T^{2} + 106.300T^{-1}$

$\Delta Gf° = 101.882 - 3.200\times10^{-3}T\ln T + 4.416\times10^{-6}T^{2} + 53.150T^{-1} - 16.982\times10^{-3}T$

631-750 K: $\Delta Hf° = 104.431 - 5.124\times10^{-3}T + 2.609\times10^{-6}T^{2} + 47.300T^{-1}$

$\Delta Gf° = 104.431 + 5.124\times10^{-3}T\ln T - 2.609\times10^{-6}T^{2} + 23.650T^{-1} - 70.182\times10^{-3}T$

750-1728 K: $\Delta Hf° = 101.521 + 1.125\times10^{-3}T - 1.293\times10^{-6}T^{2} + 360.900T^{-1}$

$\Delta Gf° = 101.521 - 1.125\times10^{-3}T\ln T + 1.293\times10^{-6}T^{2} + 180.450T^{-1} - 28.138\times10^{-3}T$

1728-2000 K: $\Delta Hf° = 101.455 - 3.104\times10^{-3}T - 0.136\times10^{-6}T^{2} + 47.300T^{-1}$

$\Delta Gf° = 101.455 + 3.104\times10^{-3}T\ln T + 0.136\times10^{-6}T^{2} + 23.650T^{-1} - 57.575\times10^{-3}T$

Source: Data from Mah (150).

NiO(c)

Nickel Oxide

[Formation: $Ni(c,1) + 0.5O_2(g) = NiO(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.590	9.080	9.080	0	-57.300	-50.573	37.071
300	10.630	9.150	9.083	.020	-57.299	-50.532	36.812
400	12.310	12.440	9.515	1.170	-57.156	-48.294	26.386
500	15.530	15.480	10.420	2.530	-56.871	-46.116	20.157
525	16.910	16.270	10.670	2.940	-56.743	-45.576	18.972
525	13.070	16.270	10.670	2.940	-56.743	-45.576	18.972
565	14.680	17.290	11.113	3.490	-56.651	-44.736	17.304
565	12.850	17.290	11.113	3.490	-56.651	-44.736	17.304
600	12.820	18.060	11.493	3.940	-56.621	-43.997	16.026
631	12.801	18.705	11.832	4.337	-56.612	-43.344	15.012
700	12.760	20.030	12.573	5.220	-56.528	-41.892	13.079
800	12.750	21.730	13.605	6.500	-56.383	-39.807	10.875
900	12.810	23.240	14.607	7.770	-56.268	-37.756	9.168
1000	12.940	24.590	15.530	9.060	-56.154	-35.699	7.802
1100	13.140	25.830	16.403	10.370	-56.042	-33.640	6.684
1200	13.380	26.990	17.248	11.690	-55.942	-31.625	5.760
1300	13.650	28.070	18.039	13.040	-55.834	-29.605	4.977
1400	13.950	29.090	18.790	14.420	-55.722	-27.586	4.306
1500	14.250	30.060	19.507	15.830	-55.604	-25.579	3.727
1600	14.540	30.990	20.196	17.270	-55.482	-23.579	3.221
1700	14.800	31.880	20.856	18.740	-55.355	-21.598	2.777
1728	14.859	32.122	21.037	19.155	-55.321	-21.030	2.660
1728	14.859	32.122	21.037	19.155	-59.421	-21.030	2.660
1800	15.010	32.730	21.491	20.230	-59.336	-19.428	2.359
1900	15.160	33.550	22.108	21.740	-59.203	-17.227	1.982
2000	15.230	34.330	22.700	23.260	-59.063	-15.017	1.641

Phase changes: 525 K, α - β transition point of NiO; $\Delta H° = 0$ kcal/mol.
565 K, β - γ transition point of NiO; $\Delta H° = 0$ kcal/mol.
631 K, Curie temperature of Ni; $\Delta H° = 0$ kcal/mol.
1728 K, melting point of Ni; $\Delta H° = 4.100$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-525 K: $Cp° = -1.511 + 31.366\times10^{-3}T + 2.443\times10^{5}T^{-2}$

$H°- H°_{298} = -1.511\times10^{-3}T + 15.683\times10^{-6}T^{2} - 2.443\times10^{2}T^{-1} - 0.124$

525-565 K: $Cp° = -8.186 + 40.260\times10^{-3}T$

$H°- H°_{298} = -8.186\times10^{-3}T + 20.130\times10^{-6}T^{2} + 1.689$

565-2000 K: $Cp° = 9.540 + 2.956\times10^{-3}T + 5.231\times10^{5}T^{-2}$

$H°- H°_{298} = 9.540\times10^{-3}T + 1.478\times10^{-6}T^{2} - 5.231\times10^{2}T^{-1} - 1.446$

NiO(c) - Continued

Formation equations (kcal/mol):

298.15-525 K: $\Delta Hf^\circ = -55.172 - 8.122\times10^{-3}T + 11.152\times10^{-6}T^2 - 207.900T^{-1}$

$\Delta Gf^\circ = -55.172 + 8.122\times10^{-3}T\ln T - 11.152\times10^{-6}T^2 - 103.950T^{-1} - 26.355\times10^{-3}T$

525-565 K: $\Delta Hf^\circ = -53.359 - 14.797\times10^{-3}T + 15.599\times10^{-6}T^2 + 36.400T^{-1}$

$\Delta Gf^\circ = -53.359 + 14.797\times10^{-3}T\ln T - 15.599\times10^{-6}T^2 + 18.200T^{-1} - 69.726\times10^{-3}T$

565-631 K: $\Delta Hf^\circ = -56.494 + 2.929\times10^{-3}T - 3.054\times10^{-6}T^2 - 486.700T^{-1}$

$\Delta Gf^\circ = -56.494 - 2.929\times10^{-3}T\ln T + 3.054\times10^{-6}T^2 - 243.350T^{-1} + 38.431\times10^{-3}T$

631-750 K: $\Delta Hf^\circ = -53.945 - 5.395\times10^{-3}T + 3.971\times10^{-6}T^2 - 545.700T^{-1}$

$\Delta Gf^\circ = -53.945 + 5.395\times10^{-3}T\ln T - 3.971\times10^{-6}T^2 - 272.850T^{-1} - 14.769\times10^{-3}T$

750-1728 K: $\Delta Hf^\circ = -56.855 + 0.854\times10^{-3}T + 0.070\times10^{-6}T^2 - 232.100T^{-1}$

$\Delta Gf^\circ = -56.855 - 0.854\times10^{-3}T\ln T - 0.070\times10^{-6}T^2 - 116.050T^{-1} + 27.274\times10^{-3}T$

1728-2000 K: $\Delta Hf^\circ = -56.921 - 3.375\times10^{-3}T + 1.227\times10^{-6}T^2 - 545.700T^{-1}$

$\Delta Gf^\circ = -56.921 + 3.375\times10^{-3}T\ln T - 1.227\times10^{-6}T^2 - 272.850T^{-1} - 2.162\times10^{-3}T$

Source: Data from Mah (150).

NiO(g)

Nickel Oxide (ideal gas)

[Formation: $Ni(c,l) + 0.5O_2(g) = NiO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.090	57.660	57.660	0	74.000	66.243	-48.557
300	8.100	57.710	57.660	.020	74.001	66.200	-48.226
400	8.640	60.120	57.995	.850	73.825	63.615	-34.757
500	9.080	62.090	58.610	1.740	73.639	61.089	-26.702
600	9.410	63.780	59.330	2.670	73.410	58.601	-21.345
631	9.484	64.256	59.560	2.963	73.314	57.840	-20.033
700	9.650	65.250	60.079	3.620	73.173	56.154	-17.532
800	9.810	66.550	60.813	4.590	73.007	53.727	-14.677
900	9.900	67.710	61.510	5.580	72.841	51.331	-12.465
1000	9.950	68.760	62.190	6.570	72.656	48.941	-10.696
1100	9.960	69.700	62.818	7.570	72.459	46.603	-9.259
1200	9.950	70.570	63.437	8.560	72.229	44.249	-8.059
1300	9.940	71.370	64.016	9.560	71.985	41.925	-7.048
1400	9.910	72.100	64.564	10.550	71.709	39.630	-6.186
1500	9.880	72.780	65.087	11.540	71.407	37.351	-5.442
1600	9.850	73.420	65.589	12.530	71.078	35.093	-4.793
1700	9.820	74.020	66.073	13.510	70.715	32.834	-4.221
1728	9.812	74.180	66.203	13.785	70.609	32.226	-4.076
1728	9.812	74.180	66.203	13.785	66.509	32.226	-4.076
1800	9.790	74.580	66.530	14.490	66.224	30.802	-3.740
1900	9.760	75.110	66.968	15.470	65.827	28.839	-3.317
2000	9.730	75.610	67.390	16.440	65.418	26.904	-2.940

Phase changes: 631 K, Curie temperature of Ni; $\Delta H° = 0$ kcal/mol.
1728 K, melting point of Ni; $\Delta H° = 4.100$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.517 + 0.368\times10^{-3}T - 1.366\times10^{5}T^{-2}$

$H°- H°_{298} = 9.517\times10^{-3}T + 0.184\times10^{-6}T^{2} + 1.366\times10^{2}T^{-1} - 3.312$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf° = 72.940 + 2.906\times10^{-3}T - 4.348\times10^{-6}T^{2} + 173.000T^{-1}$

$\Delta Gf° = 72.940 - 2.906\times10^{-3}T\ln T + 4.348\times10^{-6}T^{2} + 86.500T^{-1} - 8.174\times10^{-3}T$

631-750 K: $\Delta Hf° = 75.489 - 5.418\times10^{-3}T + 2.677\times10^{-6}T^{2} + 114.000T^{-1}$

$\Delta Gf° = 75.489 + 5.418\times10^{-3}T\ln T - 2.677\times10^{-6}T^{2} + 57.000T^{-1} - 61.374\times10^{-3}T$

750-1728 K: $\Delta Hf° = 72.579 + 0.831\times10^{-3}T - 1.224\times10^{-6}T^{2} + 427.600T^{-1}$

$\Delta Gf° = 72.579 - 0.831\times10^{-3}T\ln T + 1.224\times10^{-6}T^{2} + 213.800T^{-1} - 19.330\times10^{-3}T$

1728-2000 K: $\Delta Hf° = 72.513 - 3.398\times10^{-3}T - 0.067\times10^{-6}T^{2} + 114.000T^{-1}$

$\Delta Gf° = 72.513 + 3.398\times10^{-3}T\ln T + 0.067\times10^{-6}T^{2} + 57.000T^{-1} - 48.766\times10^{-3}T$

Source: Data from Mah (150).

Np(c,1)

Neptunium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	7.080	12.060	12.060	0
300	7.090	12.104	12.061	.013
400	8.127	14.266	12.349	.767
500	9.667	16.240	12.930	1.655
553	10.572	17.258	13.296	2.191
553*	9.400	19.681	13.296	3.531
600	9.400	20.448	13.828	3.972
700	9.400	21.897	14.880	4.912
800	9.400	23.152	15.837	5.852
849	9.400	23.711	16.275	6.313
849	8.700	25.195	16.275	7.573
900	8.700	25.703	16.795	8.017
912	8.700	25.818	16.914	8.121
912	10.850	27.178	16.914	9.361
1000	10.850	28.177	17.861	10.316
1100	10.850	29.211	18.846	11.401
1200	10.850	30.155	19.750	12.486
1300	10.850	31.024	20.585	13.571
1400	10.850	31.828	21.359	14.656
1500	10.850	32.576	22.082	15.741
1600	10.850	33.277	22.761	16.826
1700	10.850	33.934	23.398	17.911
1800	10.850	34.555	24.002	18.996
1900	10.850	35.141	24.572	20.081
2000	10.850	35.698	25.115	21.166
2100	10.850	36.227	25.631	22.251
2200	10.850	36.732	26.125	23.336
2300	10.850	37.214	26.596	24.421
2400	10.850	37.676	27.049	25.506
2500	10.850	38.119	27.483	26.591

*Data above 553 K, except temperature and enthalpy of fusion, estimated.

Phase changes: 553 K, α - β transition point of Np; ΔH° = 1.340 kcal/mol.
849 K, β - γ transition point of Np; ΔH° = 1.260 kcal/mol.
912 K, melting point of Np; ΔH° = 1.240 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-553 K: $Cp^\circ = -0.903 + 19.622\times10^{-3}T + 1.896\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = -0.903\times10^{-3}T + 9.811\times10^{-6}T^2 - 1.896\times10^{2}T^{-1} + 0.033$

553-849 K: $Cp^\circ = 9.399$

$H^\circ - H^\circ_{298} = 9.399\times10^{-3}T - 1.667$

849-912 K: $Cp^\circ = 8.698$

$H^\circ - H^\circ_{298} = 8.698\times10^{-3}T + 0.188$

912-2500 K: $Cp^\circ = 10.850$

$H^\circ - H^\circ_{298} = 10.850\times10^{-3}T - 0.534$

Source: Data from Oetting (167) who estimated data above 553 K except temperature and enthalpy of fusion.

Np(g)

Neptunium (ideal monatomic gas)

[Formation: Np(c,l) = Np(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.977	47.229	47.229	0	111.100	100.614	-73.751
300	4.977	47.260	47.230	.009	111.096	100.549	-73.249
400	5.033	48.698	47.426	.509	110.842	97.069	-53.035
500	5.166	49.834	47.798	1.018	110.463	93.666	-40.941
553	5.278	50.358	48.017	1.295	110.204	91.899	-36.319
553	5.278	50.358	48.017	1.295	108.864	91.899	-36.319
600	5.377	50.793	48.218	1.545	108.673	90.466	-32.952
700	5.650	51.642	48.648	2.096	108.284	87.462	-27.307
800	5.961	52.417	49.072	2.676	107.924	84.512	-23.087
849	6.122	52.776	49.276	2.972	107.759	83.083	-21.387
849	6.122	52.776	49.276	2.972	106.499	83.083	-21.387
900	6.289	53.138	49.484	3.289	106.372	81.681	-19.834
912	6.328	53.222	49.532	3.365	106.344	81.352	-19.495
912	6.328	53.222	49.532	3.365	105.104	81.352	-19.495
1000	6.616	53.817	49.883	3.934	104.718	79.078	-17.282
1100	6.934	54.463	50.270	4.612	104.311	76.534	-15.206
1200	7.237	55.079	50.646	5.320	103.934	74.025	-13.482
1300	7.524	55.670	51.010	6.058	103.587	71.547	-12.028
1400	7.795	56.237	51.363	6.824	103.268	69.095	-10.786
1500	8.051	56.784	51.706	7.617	102.976	66.664	-9.713
1600	8.293	57.311	52.040	8.434	102.708	64.254	-8.777
1700	8.522	57.821	52.365	9.275	102.464	61.856	-7.952
1800	8.740	58.315	52.683	10.138	102.242	59.474	-7.221
1900	8.945	58.793	52.991	11.023	102.042	57.103	-6.568
2000	9.139	59.256	53.292	11.927	101.861	54.745	-5.982
2100	9.323	59.707	53.588	12.850	101.699	52.391	-5.452
2200	9.495	60.145	53.876	13.791	101.555	50.046	-4.972
2300	9.656	60.570	54.157	14.749	101.428	47.709	-4.533
2400	9.807	60.984	54.433	15.722	101.316	45.377	-4.132
2500	9.947	61.388	54.704	16.710	101.219	43.046	-3.763

Phase changes: 553 K, α - β transition point of Np; $\Delta H° = 1.340$ kcal/mol.
849 K, β - γ transition point of Np; $\Delta H° = 1.260$ kcal/mol.
912 K, melting point of Np; $\Delta H° = 1.240$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 3.722 + 2.764\times10^{-3}T + 0.383\times10^{5}T^{-2}$

$H°- H°_{298} = 3.722\times10^{-3}T + 1.382\times10^{-6}T^{2} - 0.383\times10^{2}T^{-1} - 1.104$

Formation equations (kcal/mol):

298.15-553 K: $\Delta Hf° = 109.963 + 4.625\times10^{-3}T - 8.429\times10^{-6}T^{2} + 151.300T^{-1}$

$\Delta Gf° = 109.963 - 4.625\times10^{-3}T\ln T + 8.429\times10^{-6}T^{2} + 75.650T^{-1} - 8.368\times10^{-3}T$

553-849 K: $\Delta Hf° = 111.662 - 5.677\times10^{-3}T + 1.382\times10^{-6}T^{2} - 38.300T^{-1}$

$\Delta Gf° = 111.662 + 5.677\times10^{-3}T\ln T - 1.382\times10^{-6}T^{2} - 19.150T^{-1} - 70.767\times10^{-3}T$

849-912 K: $\Delta Hf° = 109.807 - 4.976\times10^{-3}T + 1.382\times10^{-6}T^{2} - 38.300T^{-1}$

$\Delta Gf° = 109.807 + 4.976\times10^{-3}T\ln T - 1.382\times10^{-6}T^{2} - 19.150T^{-1} - 63.854\times10^{-3}T$

912-2500 K: $\Delta Hf° = 110.530 - 7.128\times10^{-3}T + 1.382\times10^{-6}T^{2} - 38.300T^{-1}$

$\Delta Gf° = 110.530 + 7.128\times10^{-3}T\ln T - 1.382\times10^{-6}T^{2} - 19.150T^{-1} - 79.313\times10^{-3}T$

Source: Data from Oetting (167).

$O_2(g)$

Oxygen

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	7.021	49.005	49.005	0
300	7.023	49.049	49.006	.013
400	7.196	51.090	49.283	.723
500	7.431	52.721	49.813	1.454
600	7.670	54.097	50.415	2.209
700	7.883	55.296	51.029	2.987
800	8.062	56.360	51.629	3.785
900	8.211	57.319	52.209	4.599
1000	8.334	58.190	52.764	5.426
1100	8.437	58.990	53.295	6.265
1200	8.525	59.728	53.801	7.113
1300	8.601	60.413	54.283	7.969
1400	8.670	61.053	54.744	8.833
1500	8.734	61.653	55.184	9.703
1600	8.795	62.219	55.607	10.580
1700	8.853	62.754	56.012	11.462
1800	8.909	63.262	56.401	12.350
1900	8.965	63.745	56.774	13.244
2000	9.020	64.206	57.135	14.143
2100	9.075	64.648	57.482	15.048
2200	9.129	65.071	57.817	15.958
2300	9.182	65.478	58.141	16.874
2400	9.235	65.870	58.455	17.795
2500	9.287	66.248	58.760	18.721
2600	9.337	66.613	59.055	19.652
2700	9.387	66.966	59.341	20.588
2800	9.435	67.309	59.620	21.529
2900	9.482	67.641	59.891	22.475
3000	9.528	67.963	60.154	23.426

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:

$$Cp^\circ = 7.230 + 1.006\times10^{-3}T - 0.452\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 7.230\times10^{-3}T + 0.503\times10^{-6}T^{2} + 0.452\times10^{2}T^{-1} - 2.352$$

2000-3000 K:

$$Cp^\circ = 8.340 + 0.418\times10^{-3}T - 6.300\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 8.340\times10^{-3}T + 0.209\times10^{-6}T^{2} + 6.300\times10^{2}T^{-1} - 3.688$$

Source: Data from JANAF (52).

O(g)

Oxygen (ideal monatomic gas)

[Formation: $0.5O_2(g) = O(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	5.237	38.468	38.468	0	59.554	55.390	-40.602
300	5.234	38.500	38.468	.010	59.557	55.365	-40.333
400	5.134	39.991	38.671	.528	59.721	53.942	-29.472
500	5.081	41.130	39.054	1.038	59.865	52.480	-22.939
600	5.049	42.053	39.480	1.544	59.993	50.991	-18.573
700	5.029	42.830	39.904	2.048	60.109	49.481	-15.448
800	5.015	43.501	40.313	2.550	60.211	47.955	-13.100
900	5.006	44.091	40.701	3.051	60.306	46.417	-11.271
1000	4.999	44.618	41.066	3.552	60.393	44.870	-9.806
1100	4.994	45.094	41.411	4.051	60.472	43.314	-8.606
1200	4.990	45.528	41.736	4.550	60.548	41.751	-7.604
1300	4.987	45.927	42.043	5.049	60.619	40.182	-6.755
1400	4.984	46.297	42.334	5.548	60.685	38.607	-6.027
1500	4.982	46.641	42.610	6.046	60.748	37.027	-5.395
1600	4.981	46.962	42.872	6.544	60.808	35.444	-4.841
1700	4.979	47.264	43.122	7.042	60.865	33.857	-4.353
1800	4.978	47.549	43.360	7.540	60.919	32.267	-3.918
1900	4.978	47.818	43.587	8.038	60.970	30.674	-3.528
2000	4.978	48.073	43.805	8.536	61.019	29.079	-3.178
2100	4.978	48.316	44.015	9.033	61.063	27.480	-2.860
2200	4.978	48.548	44.216	9.531	61.106	25.878	-2.571
2300	4.980	48.769	44.409	10.029	61.146	24.277	-2.307
2400	4.981	48.981	44.595	10.527	61.184	22.673	-2.065
2500	4.983	49.184	44.774	11.025	61.219	21.069	-1.842
2600	4.986	49.380	44.948	11.524	61.252	19.461	-1.636
2700	4.990	49.568	45.115	12.023	61.283	17.854	-1.445
2800	4.994	49.750	45.278	12.522	61.312	16.244	-1.268
2900	4.999	49.925	45.435	13.021	61.338	14.634	-1.103
3000	5.004	50.094	45.587	13.522	61.363	13.025	-.949

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 4.987 - 0.006\times10^{-3}T + 0.224\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.987\times10^{-3}T - 0.003\times10^{-6}T^2 - 0.224\times10^{2}T^{-1} - 1.411$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 59.318 + 1.372\times10^{-3}T - 0.254\times10^{-6}T^2 - 45.000T^{-1}$

$\Delta Gf^\circ = 59.318 - 1.372\times10^{-3}T\ln T + 0.254\times10^{-6}T^2 - 22.500T^{-1} - 5.181\times10^{-3}T$

2000-3000 K: $\Delta Hf^\circ = 59.987 + 0.817\times10^{-3}T - 0.108\times10^{-6}T^2 - 337.400T^{-1}$

$\Delta Gf^\circ = 59.987 - 0.817\times10^{-3}T\ln T + 0.108\times10^{-6}T^2 - 168.700T^{-1} - 9.403\times10^{-3}T$

Source: Data from JANAF (52).

$O_3(g)$

Oxygen (ideal triatomic gas), Ozone

[Formation: $1.5O_2(g) = O_3(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.378	57.080	57.080	0	34.200	39.098	-28.659
300	9.400	57.138	57.081	.017	34.197	39.128	-28.504
400	10.455	59.992	57.462	1.012	34.128	40.785	-22.283
500	11.296	62.419	58.217	2.101	34.120	42.451	-18.555
600	11.916	64.536	59.098	3.263	34.150	44.115	-16.069
700	12.369	66.409	60.010	4.479	34.199	45.773	-14.291
800	12.704	68.083	60.917	5.733	34.256	47.421	-12.955
900	12.956	69.595	61.798	7.017	34.319	49.064	-11.914
1000	13.151	70.971	62.648	8.323	34.384	50.698	-11.080
1100	13.303	72.232	63.463	9.646	34.449	52.327	-10.396
1200	13.426	73.395	64.243	10.982	34.513	53.949	-9.825
1300	13.526	74.473	64.988	12.330	34.577	55.567	-9.342
1400	13.611	75.479	65.703	13.687	34.638	57.178	-8.926
1500	13.682	76.420	66.385	15.052	34.698	58.787	-8.565
1600	13.743	77.305	67.041	16.423	34.753	60.391	-8.249
1700	13.796	78.140	67.669	17.800	34.807	61.992	-7.969
1800	13.843	78.930	68.273	19.182	34.857	63.590	-7.721
1900	13.885	79.680	68.854	20.569	34.903	65.184	-7.498
2000	13.922	80.393	69.413	21.959	34.944	66.777	-7.297

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.697 + 1.460\times10^{-3}T - 2.448\times10^{5}T^{-2}$

$H°- H°_{298} = 11.697\times10^{-3}T + 0.730\times10^{-6}T^{2} + 2.448\times10^{2}T^{-1} - 4.373$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 33.354 + 0.852\times10^{-3}T - 0.024\times10^{-6}T^{2} + 177.000T^{-1}$

$\Delta Gf° = 33.354 - 0.852\times10^{-3}T\ln T + 0.024\times10^{-6}T^{2} + 88.500T^{-1} + 23.115\times10^{-3}T$

Source: Data from JANAF (51).

Os(c)

Osmium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.905	7.800	7.800	0
300	5.906	7.837	7.800	.011
400	5.998	9.548	8.033	.606
500	6.089	10.896	8.476	1.210
600	6.180	12.015	8.975	1.824
700	6.271	12.977	9.481	2.447
800	6.362	13.817	9.970	3.078
900	6.453	14.572	10.440	3.719
1000	6.544	15.256	10.887	4.369
1100	6.635	15.884	11.313	5.028
1200	6.726	16.465	11.719	5.695
1300	6.817	17.007	12.105	6.372
1400	6.908	17.516	12.474	7.059
1500	6.999	17.995	12.826	7.754
1600	7.090	18.450	13.163	8.459
1700	7.181	18.883	13.488	9.172
1800	7.272	19.296	13.799	9.895
1900	7.363	19.691	14.098	10.627
2000	7.454	20.071	14.387	11.367

Phase change: 3300 K, melting point of Os; ΔH° = 7.6 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 5.636 + 0.908 \times 10^{-3} T$

$H^\circ - H^\circ_{298} = 5.636 \times 10^{-3} T + 0.454 \times 10^{-6} T^2 - 1.721$

Source: Data from Hultgren (99).

Os(g)

Osmium (ideal monatomic gas)

[Formation: Os(c) = Os(g)]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	46.000	46.000	0	189.000	177.611	-130.190
300	4.968	46.031	46.001	.009	188.998	177.540	-129.336
400	4.974	47.461	46.196	.506	188.900	173.735	-94.923
500	4.995	48.572	46.562	1.005	188.795	169.957	-74.287
600	5.043	49.487	46.977	1.506	188.682	166.199	-60.537
700	5.122	50.270	47.393	2.014	188.567	162.462	-50.722
800	5.231	50.961	47.796	2.532	188.454	158.739	-43.365
900	5.366	51.584	48.183	3.061	188.342	155.031	-37.646
1000	5.522	52.158	48.552	3.606	188.237	151.335	-33.074
1100	5.691	52.692	48.905	4.166	188.138	147.649	-29.335
1200	5.866	53.195	49.242	4.744	188.049	143.973	-26.221
1300	6.041	53.671	49.564	5.339	187.967	140.304	-23.587
1400	6.211	54.125	49.874	5.952	187.893	136.640	-21.330
1500	6.372	54.559	50.172	6.581	187.827	132.981	-19.375
1600	6.521	54.975	50.459	7.226	187.767	129.327	-17.665
1700	6.658	55.374	50.736	7.885	187.713	125.678	-16.157
1800	6.782	55.759	51.005	8.557	187.662	122.029	-14.816
1900	6.895	56.128	51.264	9.241	187.614	118.384	-13.617
2000	6.998	56.485	51.517	9.936	187.569	114.741	-12.538

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 3.985 + 1.550\times10^{-3}T + 0.463\times10^{5}T^{-2}$

$H°- H°_{298} = 3.985\times10^{-3}T + 0.775\times10^{-6}T^{2} - 0.463\times10^{2}T^{-1} - 1.102$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 189.619 - 1.651\times10^{-3}T + 0.321\times10^{-6}T^{2} - 46.300T^{-1}$

$\Delta Gf° = 189.619 + 1.651\times10^{-3}T\ln T - 0.321\times10^{-6}T^{2} - 23.150T^{-1} - 49.327\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). All other data from Hilsenrath (94).

P[c,1,1/4P_4(g)]

White Phosphorus

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.698	9.820	9.820	0
300	5.704	9.855	9.820	.011
317.3	5.820	10.179	9.832	.110
317.3	6.292	10.674	9.832	.267
400*	6.292	12.131	10.163	.787
500	6.292	13.535	10.703	1.416
550	6.292	14.109	10.962	1.731
550	4.627	19.396	10.962	4.639
600	4.684	19.803	11.683	4.872
700	4.756	20.531	12.897	5.344
800	4.804	21.169	13.892	5.822
900	4.837	21.737	14.733	6.304
1000	4.861	22.248	15.459	6.789
1100	4.880	22.712	16.097	7.276
1200	4.894	23.137	16.666	7.765
1300	4.904	23.529	17.179	8.255
1400	4.913	23.893	17.646	8.746
1500	4.920	24.232	18.073	9.238
1600	4.926	24.550	18.469	9.730
1700	4.931	24.849	18.835	10.223
1800	4.935	25.131	19.178	10.716
1900	4.938	25.398	19.498	11.210
2000	4.941	25.651	19.799	11.703

*Data extrapolated 400 - 550 K.

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to P_4(g); ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-317.3 K: $Cp^\circ = 3.799 + 6.370\times10^{-3}T$

$H^\circ - H^\circ_{298} = 3.799\times10^{-3}T + 3.185\times10^{-6}T^2 - 1.416$

317.3-550 K: $Cp^\circ = 6.292$

$H^\circ - H^\circ_{298} = 6.292\times10^{-3}T - 1.729$

550-2000 K: $Cp^\circ = 4.954 + 0.008\times10^{-3}T - 1.003\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.954\times10^{-3}T + 0.004\times10^{-6}T^2 + 1.003\times10^{2}T^{-1} + 1.731$

Sources: Entropy at 298 K of P(white) from CODATA (36). Data for P(white,1) from Hultgren (99) who extrapolated 400 - 550 K. Enthalpy of formation at 298 K for P_4(g) from Parker (181). Other data for P_4(g) from JANAF (51).

P(red)

Red Phosphorus (triclinic)

[Formation: $P(c,1,1/4P_4(g)) = P(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^{\circ}_{298})/T$	$H°-H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	5.069	5.460	5.460	0	-4.200	-2.900	2.126
300	5.082	5.491	5.461	.009	-4.202	-2.893	2.107
317.3	5.161	5.778	5.471	.098	-4.212	-2.816	1.940
317.3	5.161	5.778	5.471	.098	-4.369	-2.816	1.940
400	5.540	7.019	5.664	.542	-4.445	-2.400	1.311
500	5.852	8.292	6.068	1.112	-4.504	-1.882	.823
550	6.009	8.856	6.295	1.409	-4.522	-1.633	.649
550	6.009	8.856	6.295	1.409	-7.430	-1.633	.649
600	6.165	9.386	6.531	1.713	-7.359	-1.109	.404
700	6.500	10.361	7.010	2.346	-7.198	-.079	.025

Phase changes: 317.3 K, melting point of P(white); $\Delta H° = 0.157$ kcal/mol.
550 K, boiling point of P(white); $\Delta H° = 2.908$ kcal/mol of P(white).
704 K, sublimation point of P(red); $\Delta H° = 7.1$ kcal/mol of P(red).

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 4.764 + 2.544\times10^{-3}T - 0.404\times10^{5}T^{-2}$

$H°-H^{\circ}_{298} = 4.764\times10^{-3}T + 1.272\times10^{-6}T^{2} + 0.404\times10^{2}T^{-1} - 1.669$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -4.453 + 0.965\times10^{-3}T - 1.913\times10^{-6}T^{2} + 40.400T^{-1}$

$\Delta Gf° = -4.453 - 0.965\times10^{-3}T\ln T + 1.913\times10^{-6}T^{2} + 20.200T^{-1} + 9.910\times10^{-3}T$

317.3-550 K: $\Delta Hf° = -4.140 - 1.528\times10^{-3}T + 1.272\times10^{-6}T^{2} + 40.400T^{-1}$

$\Delta Gf° = -4.140 + 1.528\times10^{-3}T\ln T - 1.272\times10^{-6}T^{2} + 20.200T^{-1} - 4.427\times10^{-3}T$

550-700 K: $\Delta Hf° = -7.600 - 0.190\times10^{-3}T + 1.268\times10^{-6}T^{2} - 59.900T^{-1}$

$\Delta Gf° = -7.600 + 0.190\times10^{-3}T\ln T - 1.268\times10^{-6}T^{2} - 29.950T^{-1} + 10.471\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from Hultgren (99).

P(g)

Phosphorus (ideal monatomic gas)

[Formation: $P(c,1,1/4P_4(g)) = P(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^{\circ}_{298})/T$	$H°-H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	4.968	38.980	38.980	0	75.620	66.926	-49.057
300	4.968	39.011	38.981	.009	75.618	66.871	-48.715
317.3	4.968	39.290	38.990	.095	75.605	66.368	-45.712
317.3	4.968	39.290	38.990	.095	75.448	66.368	-45.712
400	4.968	40.440	39.175	.506	75.339	64.015	-34.976
500	4.968	41.548	39.542	1.003	75.207	61.201	-26.750
550	4.968	42.022	39.746	1.252	75.141	59.788	-23.757
550	4.968	42.022	39.746	1.252	72.233	59.788	-23.757
600	4.968	42.454	39.954	1.500	72.248	58.657	-21.366
700	4.968	43.220	40.369	1.996	72.272	56.390	-17.605
800	4.968	43.883	40.767	2.493	72.291	54.120	-14.785
900	4.968	44.469	41.147	2.990	72.306	51.847	-12.590
1000	4.968	44.992	41.505	3.487	72.318	49.574	-10.834
1100	4.969	45.466	41.844	3.984	72.328	47.299	-9.397
1200	4.969	45.898	42.164	4.481	72.336	45.023	-8.200
1300	4.971	46.296	42.467	4.978	72.343	42.746	-7.186
1400	4.974	46.664	42.753	5.475	72.349	40.470	-6.318
1500	4.979	47.008	43.027	5.972	72.354	38.190	-5.564
1600	4.987	47.329	43.285	6.471	72.361	35.915	-4.906
1700	4.999	47.632	43.532	6.970	72.367	33.636	-4.324
1800	5.015	47.918	43.767	7.471	72.375	31.358	-3.807
1900	5.036	48.190	43.994	7.973	72.383	29.078	-3.345
2000	5.062	48.449	44.210	8.478	72.395	26.799	-2.928

Phase changes: 317.3 K, melting point of P; $\Delta H° = 0.157$ Kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H° = 2.908$ kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.951 + 0.022\times10^{-3}T + 0.009\times10^{5}T^{-2}$

$H°-H^{\circ}_{298} = 4.951\times10^{-3}T + 0.011\times10^{-6}T^{2} - 0.009\times10^{2}T^{-1} - 1.474$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = 75.562 + 1.152\times10^{-3}T - 3.174\times10^{-6}T^{2} - 0.900T^{-1}$

$\Delta Gf° = 75.562 - 1.152\times10^{-3}T\ln T + 3.174\times10^{-6}T^{2} - 0.450T^{-1} - 23.342\times10^{-3}T$

317.3-550 K: $\Delta Hf° = 75.875 - 1.341\times10^{-3}T + 0.011\times10^{-6}T^{2} - 0.900T^{-1}$

$\Delta Gf° = 75.875 + 1.341\times10^{-3}T\ln T - 0.011\times10^{-6}T^{2} - 0.450T^{-1} - 37.678\times10^{-3}T$

550-2000 K: $\Delta Hf° = 72.415 - 0.003\times10^{-3}T + 0.007\times10^{-6}T^{2} - 101.200T^{-1}$

$\Delta Gf° = 72.415 + 0.003\times10^{-3}T\ln T - 0.007\times10^{-6}T^{2} - 50.600T^{-1} - 22.781\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (181). All other data from JANAF (51).

$P_2(g)$

Phosphorus (ideal diatomic gas)

[Formation: $2P(c,1,1/4P_4(g)) = P_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.657	52.110	52.110	0	34.370	24.689	-18.097
300	7.665	52.157	52.110	.014	34.362	24.628	-17.941
317.3	7.732	52.589	52.125	.147	34.297	24.070	-16.579
317.3	7.732	52.589	52.125	.147	33.983	24.070	-16.579
400	8.050	54.418	52.416	.801	33.597	21.535	-11.766
500	8.311	56.244	53.004	1.620	33.158	18.571	-8.117
550	8.398	57.041	53.336	2.038	32.946	17.093	-6.792
550	8.398	57.041	53.336	2.038	27.130	17.093	-6.792
600	8.485	57.776	53.676	2.460	27.086	16.184	-5.895
700	8.604	59.093	54.357	3.315	26.997	14.375	-4.488
800	8.690	60.248	55.023	4.180	26.906	12.578	-3.436
900	8.752	61.275	55.662	5.052	26.814	10.793	-2.621
1000	8.800	62.200	56.270	5.930	26.722	9.018	-1.971
1100	8.836	63.041	56.848	6.812	26.630	7.251	-1.441
1200	8.868	63.811	57.397	7.697	26.537	5.493	-1.000
1300	8.893	64.522	57.918	8.585	26.445	3.742	-.629
1400	8.914	65.182	58.413	9.476	26.354	2.000	-.312
1500	8.933	65.797	58.885	10.368	26.262	0.263	-.038
1600	8.949	66.374	59.335	11.262	26.172	-1.466	.200
1700	8.963	66.917	59.765	12.158	26.082	-3.190	.410
1800	8.976	67.430	60.177	13.055	25.993	-4.909	.596
1900	8.987	67.916	60.572	13.953	25.903	-6.625	.762
2000	8.998	68.377	60.951	14.852	25.816	-8.334	.911

Phase changes: 317.3 K, melting point of P; $\Delta H° = 0.157$ kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H° = 2.908$ kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.571 + 0.270\times10^{-3}T - 0.884\times10^{5}T^{-2}$

$H°- H°_{298} = 8.571\times10^{-3}T + 0.135\times10^{-6}T^2 + 0.884\times10^{2}T^{-1} - 2.864$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = 34.338 + 0.973\times10^{-3}T - 6.235\times10^{-6}T^2 + 88.400T^{-1}$

$\Delta Gf° = 34.338 - 0.973\times10^{-3}T\ln T + 6.235\times10^{-6}T^2 + 44.200T^{-1} - 29.174\times10^{-3}T$

317.3-550 K: $\Delta Hf° = 34.964 - 4.013\times10^{-3}T + 0.135\times10^{-6}T^2 + 88.400T^{-1}$

$\Delta Gf° = 34.964 + 4.013\times10^{-3}T\ln T - 0.135\times10^{-6}T^2 + 44.200T^{-1} - 57.847\times10^{-3}T$

550-2000 K: $\Delta Gf° = 28.044 - 1.337\times10^{-3}T + 0.127\times10^{-6}T^2 - 112.200T^{-1}$

$\Delta Gf° = 28.044 + 1.337\times10^{-3}T\ln T - 0.127\times10^{-6}T^2 - 56.100T^{-1} - 28.051\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (181). All other data from JANAF (51).

$P_4(g)$

Phosphorus (ideal tetratomic gas)

[Formation: $4P(c,1,1/4P_4(g)) = P_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	16.051	66.893	66.893	0	14.125	5.892	-4.319
300	16.088	66.992	66.893	.030	14.111	5.839	-4.254
317.3	16.334	67.901	66.922	.310	13.995	5.370	-3.699
317.3	16.334	67.901	66.922	.310	13.367	5.370	-3.699
400	17.510	71.837	67.544	1.717	12.694	3.369	-1.841
500	18.281	75.835	68.815	3.510	11.971	1.124	-0.491
550	18.508	77.592	69.534	4.432	11.632	0	0
550	18.508	77.592	69.534	4.432	0	0	0
600	18.735	79.212	70.274	5.363	0	0	0
700	19.022	82.123	71.763	7.252	0	0	0
800	19.214	84.676	73.221	9.164	0	0	0
900	19.348	86.947	74.621	11.093	0	0	0
1000	19.445	88.991	75.958	13.033	0	0	0
1100	19.518	90.848	77.229	14.981	0	0	0
1200	19.574	92.549	78.436	16.936	0	0	0
1300	19.617	94.117	79.582	18.895	0	0	0
1400	19.652	95.572	80.673	20.859	0	0	0
1500	19.680	96.929	81.712	22.826	0	0	0
1600	19.703	98.200	82.703	24.795	0	0	0
1700	19.722	99.395	83.650	26.766	0	0	0
1800	19.738	100.523	84.557	28.739	0	0	0
1900	19.752	101.591	85.426	30.714	0	0	0
2000	19.764	102.604	86.259	32.689	0	0	0

Phase changes: 317.3 K, melting point of P; $\Delta H° = 0.157$ kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H° = 2.908$ kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.434 + 0.258\times10^{-3}T - 3.075\times10^{5}T^{-2}$

$H°-H°_{298} = 19.434\times10^{-3}T + 0.129\times10^{-6}T^{2} + 3.075\times10^{2}T^{-1} - 6.837$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = 12.951 + 4.238\times10^{-3}T - 12.611\times10^{-6}T^{2} + 307.500T^{-1}$

$\Delta Gf° = 12.951 - 4.238\times10^{-3}T\ln T + 12.611\times10^{-6}T^{2} + 153.750T^{-1} - 5.019\times10^{-3}T$

317.3-550 K: $\Delta Hf° = 14.205 - 5.734\times10^{-3}T + 0.129\times10^{-6}T^{2} + 307.500T^{-1}$

$\Delta Gf° = 14.205 + 5.734\times10^{-3}T\ln T - 0.129\times10^{-6}T^{2} + 153.750T^{-1} - 62.364\times10^{-3}T$

550-2000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Sources: Enthalpy of formation at 298 K from Parker (181). All other data from JANAF (51).

PO(g)

Phosphorus Oxide (ideal gas)

[Formation: $P(c,1,1/4P_4(g)) + 0.5O_2(g) = PO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.591	53.218	53.218	0	-5.630	-11.264	8.256
300	7.592	53.265	53.218	.014	-5.634	-11.299	8.231
317.3	7.615	53.691	53.233	.146	-5.662	-11.624	8.006
317.3	7.615	53.691	53.233	.146	-5.819	-11.624	8.006
400	7.727	55.464	53.517	.779	-6.000	-13.115	7.165
500	7.933	57.210	54.086	1.562	-6.211	-14.868	6.499
550	8.030	57.971	54.405	1.961	-6.314	-15.744	6.256
550	8.030	57.971	54.405	1.961	-9.222	-15.744	6.256
600	8.127	58.674	54.732	2.365	-9.242	-16.335	5.950
700	8.288	59.939	55.388	3.186	-9.281	-17.513	5.468
800	8.416	61.055	56.029	4.021	-9.324	-18.688	5.105
900	8.517	62.052	56.643	4.868	-9.366	-19.855	4.821
1000	8.598	62.954	57.230	5.724	-9.408	-21.019	4.594
1100	8.662	63.776	57.788	6.587	-9.451	-22.177	4.406
1200	8.715	64.532	58.319	7.456	-9.496	-23.333	4.249
1300	8.759	65.232	58.824	8.330	-9.540	-24.485	4.116
1400	8.796	65.882	59.305	9.208	-9.585	-25.632	4.001
1500	8.827	66.490	59.764	10.089	-9.631	-26.778	3.901
1600	8.854	67.061	60.203	10.973	-9.677	-27.919	3.814
1700	8.878	67.598	60.622	11.860	-9.724	-29.056	3.735
1800	8.899	68.106	61.023	12.749	-9.772	-30.191	3.666
1900	8.917	68.588	61.410	13.639	-9.823	-31.326	3.603
2000	8.934	69.046	61.780	14.532	-9.873	-32.456	3.547

Phase changes: 317.3 K, melting point of P; $\Delta H° = 0.157$ kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H° = 2.908$ kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.879 + 0.646\times10^{-3}T - 0.428\times10^{5}T^{-2}$

$H°- H°_{298} = 7.879\times10^{-3}T + 0.323\times10^{-6}T^{2} + 0.428\times10^{2}T^{-1} - 2.521$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -5.560 + 0.465\times10^{-3}T - 3.114\times10^{-6}T^{2} + 20.200T^{-1}$

$\Delta Gf° = -5.560 - 0.465\times10^{-3}T\ln T + 3.114\times10^{-6}T^{2} + 10.100T^{-1} - 17.524\times10^{-3}T$

317.3-550 K: $\Delta Hf° = -5.246 - 2.028\times10^{-3}T + 0.072\times10^{-6}T^{2} + 20.200T^{-1}$

$\Delta Gf° = -5.246 + 2.028\times10^{-3}T\ln T - 0.072\times10^{-6}T^{2} + 10.100T^{-1} - 31.860\times10^{-3}T$

550-2000 K: $\Delta Hf° = -8.707 - 0.690\times10^{-3}T + 0.068\times10^{-6}T^{2} - 80.100T^{-1}$

$\Delta Gf° = -8.707 + 0.690\times10^{-3}T\ln T - 0.068\times10^{-6}T^{2} - 40.050T^{-1} - 16.963\times10^{-3}T$

Source: Data from JANAF (51). Enthalpy of formation based on P(white).

$PO_2(g)$

Phosphorus Dioxide (ideal gas)

[Formation: $P(c,1,1/4P_4(g)) + O_2(g) = PO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.897	60.607	60.607	0	-75.200	-75.731	55.512
300	9.917	60.668	60.608	.018	-75.206	-75.735	55.172
317.3	10.089	61.229	60.627	.191	-75.254	-75.763	52.184
317.3	10.089	61.229	60.627	.191	-75.411	-75.763	52.184
400	10.913	63.663	61.008	1.062	-75.648	-75.825	41.428
500	11.659	66.183	61.799	2.192	-75.878	-75.841	33.150
550	11.924	67.309	62.249	2.783	-75.976	-75.847	30.138
550	11.924	67.309	62.249	2.783	-78.884	-75.847	30.138
600	12.189	68.358	62.715	3.386	-78.895	-75.570	27.526
700	12.566	70.267	63.660	4.625	-78.906	-75.014	23.420
800	12.837	71.964	64.594	5.896	-78.911	-74.459	20.341
900	13.038	73.488	65.499	7.190	-78.913	-73.902	17.946
1000	13.188	74.870	66.368	8.502	-78.913	-73.345	16.029
1100	13.304	76.132	67.198	9.827	-78.914	-72.787	14.461
1200	13.395	77.294	67.992	11.162	-78.916	-72.231	13.155
1300	13.467	78.369	68.750	12.505	-78.919	-71.674	12.049
1400	13.525	79.369	69.473	13.855	-78.924	-71.116	11.102
1500	13.573	80.304	70.164	15.210	-78.931	-70.559	10.280
1600	13.612	81.181	70.825	16.569	-78.941	-70.000	9.561
1700	13.645	82.008	71.460	17.932	-78.953	-69.441	8.927
1800	13.673	82.788	72.067	19.298	-78.968	-68.879	8.363
1900	13.697	83.528	72.651	20.666	-78.988	-68.320	7.858
2000	13.717	84.231	73.213	22.037	-79.009	-67.757	7.404

Phase changes: 317.3 K, melting point of P; $\Delta H°$ = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H°$ = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.337 + 0.900\times10^{-3}T - 2.407\times10^{5}T^{-2}$

$H°- H°_{298} = 12.337\times10^{-3}T + 0.450\times10^{-6}T^{2} + 2.407\times10^{2}T^{-1} - 4.526$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -75.958 + 1.308\times10^{-3}T - 3.238\times10^{-6}T^{2} + 195.500T^{-1}$

$\Delta Gf° = -75.958 - 1.308\times10^{-3}T\ln T + 3.238\times10^{-6}T^{2} + 97.750T^{-1} + 6.147\times10^{-3}T$

317.3-550 K: $\Delta Hf° = -75.644 - 1.185\times10^{-3}T - 0.053\times10^{-6}T^{2} + 195.500T^{-1}$

$\Delta Gf° = -75.644 + 1.185\times10^{-3}T\ln T + 0.053\times10^{-6}T^{2} + 97.750T^{-1} - 8.189\times10^{-3}T$

550-2000 K: $\Delta Hf° = -79.105 + 0.153\times10^{-3}T - 0.057\times10^{-6}T^{2} + 95.200T^{-1}$

$\Delta Gf° = -79.105 - 0.153\times10^{-3}T\ln T + 0.057\times10^{-6}T^{2} + 47.600T^{-1} + 6.709\times10^{-3}T$

Source: Data from JANAF (51). Enthalpy of formation based on P(white).

$(P_2O_3)_2(g)$

Dimeric Diphosphorus Trioxide (ideal gas)

[Formation: $4P(c,1,1/4P_4(g)) + 3O_2(g) = (P_2O_3)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	34.402	82.584	82.584	0	-529.200	-498.279	365.243
300	34.556	82.798	82.585	.064	-529.219	-498.088	362.852
317.3	35.700	84.767	82.650	.672	-529.373	-496.285	341.826
317.3	35.700	84.767	82.650	.672	-530.001	-496.285	341.826
400	41.168	93.719	84.029	3.876	-530.641	-487.411	266.306
500	45.319	103.386	86.954	8.216	-531.010	-476.552	208.298
550	46.658	107.784	88.648	10.525	-531.085	-471.159	187.219
550	46.658	107.784	88.648	10.525	-542.717	-471.159	187.219
600	47.996	111.902	90.417	12.891	-542.424	-464.663	169.251
700	49.789	119.444	94.035	17.786	-541.751	-451.753	141.042
800	51.036	126.179	97.640	22.831	-541.012	-438.950	119.914
900	51.931	132.244	101.154	27.981	-540.232	-426.237	103.503
1000	52.594	137.752	104.543	33.209	-539.425	-413.615	90.394
1100	53.096	142.789	107.794	38.495	-538.604	-401.072	79.685
1200	53.485	147.427	110.906	43.825	-537.774	-388.608	70.774
1300	53.793	151.720	113.882	49.189	-536.938	-376.213	63.246
1400	54.040	155.716	116.730	54.581	-536.102	-363.881	56.804
1500	54.241	159.451	119.454	59.996	-535.265	-351.611	51.229
1600	54.406	162.958	122.065	65.428	-534.432	-339.394	46.358
1700	54.544	166.260	124.568	70.876	-533.602	-327.225	42.067
1800	54.661	169.381	126.972	76.336	-532.778	-315.106	38.259
1900	54.760	172.339	129.283	81.807	-531.965	-303.038	34.857
2000	54.845	175.150	131.506	87.288	-531.153	-291.009	31.800

Phase changes: 317.3 K, melting point of P; $\Delta H°$ = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H°$ = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 50.372 + 3.046\times10^{-3}T - 15.003\times10^{5}T^{-2}$

$H°- H°_{298} = 50.372\times10^{-3}T + 1.523\times10^{-6}T^{2} + 15.003\times10^{2}T^{-1} - 20.186$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -536.667 + 13.486\times10^{-3}T - 12.726\times10^{-6}T^{2} + 1364.700T^{-1}$

$\Delta Gf° = -536.667 - 13.486\times10^{-3}T\ln T + 12.726\times10^{-6}T^{2} + 682.350T^{-1} + 194.122\times10^{-3}T$

317.3-550 K: $\Delta Hf° = -535.413 + 3.514\times10^{-3}T + 0.014\times10^{-6}T^{2} + 1364.700T^{-1}$

$\Delta Gf° = -535.413 - 3.514\times10^{-3}T\ln T - 0.014\times10^{-6}T^{2} + 682.350T^{-1} + 136.777\times10^{-3}T$

550-2000 K: $\Delta Hf° = -549.255 + 8.866\times10^{-3}T - 0.002\times10^{-6}T^{2} + 963.500T^{-1}$

$\Delta Gf° = -549.255 - 8.866\times10^{-3}T\ln T + 0.002\times10^{-6}T^{2} + 481.750T^{-1} + 196.368\times10^{-3}T$

Source: Data from JANAF (51). Enthalpy of formation based on P(white).

$(P_2O_5)_2(c,g)$

Dimeric Diphosphorus Pentoxide

[Formation: $4P(c,l,1/4P_4(g)) + 5O_2(g) = (P_2O_5)_2(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	50.600	54.680	54.680	0	-719.400	-650.937	477.144
300	50.830	54.994	54.681	.094	-719.415	-650.514	473.893
317.3	52.797	57.899	54.778	.990	-719.523	-646.533	445.313
317.3	52.797	57.899	54.778	.990	-720.151	-646.533	445.313
400*	62.200	71.218	56.816	5.761	-720.402	-627.300	342.736
500	71.700	86.135	61.209	12.463	-719.871	-604.066	264.034
550	76.000	93.182	63.794	16.163	-719.303	-592.568	235.462
550	76.000	93.182	63.794	16.163	-730.935	-592.568	235.462
600	80.300	99.982	66.530	20.071	-729.862	-580.033	211.274
631	82.700	104.082	68.266	22.600	-729.109	-572.305	198.218
631	66.006	138.789	68.266	44.500	-707.209	-572.305	198.218
700	68.149	145.757	75.567	49.133	-706.578	-557.585	174.084
800	70.399	155.011	84.929	56.066	-705.547	-536.375	146.529
900	72.067	163.404	93.188	63.194	-704.417	-515.292	125.128
1000	73.329	171.066	100.600	70.466	-703.220	-494.344	108.037
1100	74.304	178.102	107.329	77.850	-701.979	-473.513	94.077
1200	75.069	184.602	113.502	85.320	-700.705	-452.802	82.465
1300	75.681	190.635	119.205	92.859	-699.406	-432.196	72.658
1400	76.175	196.263	124.512	100.452	-698.097	-411.693	64.267
1500	76.581	201.532	129.471	108.091	-696.776	-391.284	57.009
1600	76.918	206.486	134.132	115.766	-695.454	-370.960	50.670
1700	77.200	211.158	138.527	123.473	-694.129	-350.715	45.087
1800	77.439	215.577	142.685	131.205	-692.809	-330.546	40.133
1900	77.642	219.770	146.634	138.959	-691.501	-310.462	35.711
2000	77.817	223.757	150.391	146.733	-690.194	-290.440	31.737

*Data extrapolated 374 - 631 K.

Phase changes: 317.3 K, melting point of P; $\Delta H° = 0.157$ kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H° = 2.908$ kcal/mol of P.
631 K, sublimation point of $(P_2O_5)_2$; $\Delta H° = 21.900$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-631 K:
$$Cp° = 33.597 + 81.148\times10^{-3}T - 6.393\times10^{5}T^{-2}$$
$$H°- H°_{298} = 33.597\times10^{-3}T + 40.574\times10^{-6}T^{2} + 6.393\times10^{2}T^{-1} - 15.768$$

631-2000 K:
$$Cp° = 75.592 + 1.978\times10^{-3}T - 43.137\times10^{5}T^{-2}$$
$$H°- H°_{298} = 75.592\times10^{-3}T + 0.989\times10^{-6}T^{2} + 43.137\times10^{2}T^{-1} - 10.429$$

Formation equations (kcal/mol):

298.15-317.3 K:
$$\Delta Hf° = -717.745 - 17.749\times10^{-3}T + 25.319\times10^{-6}T^{2} + 413.300T^{-1}$$
$$\Delta Gf° = -717.745 + 17.749\times10^{-3}T\ln T - 25.319\times10^{-6}T^{2} + 206.650T^{-1} + 128.172\times10^{-3}T$$

317.3-550 K:
$$\Delta Hf° = -716.492 - 27.721\times10^{-3}T + 38.059\times10^{-6}T^{2} + 413.300T^{-1}$$
$$\Delta Gf° = -716.492 + 27.721\times10^{-3}T\ln T - 38.059\times10^{-6}T^{2} + 206.650T^{-1} + 70.827\times10^{-3}T$$

550-631 K:
$$\Delta Hf° = -730.333 - 22.369\times10^{-3}T + 38.043\times10^{-6}T^{2} + 12.100T^{-1}$$
$$\Delta Gf° = -730.333 + 22.369\times10^{-3}T\ln T - 38.043\times10^{-6}T^{2} + 6.050T^{-1} + 130.418\times10^{-3}T$$

631-2000 K:
$$\Delta Hf° = -724.994 + 19.626\times10^{-3}T - 1.542\times10^{-6}T^{2} + 3686.500T^{-1}$$
$$\Delta Gf° = -724.994 - 19.626\times10^{-3}T\ln T + 1.542\times10^{-6}T^{2} + 1843.250T^{-1} + 363.118\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Parker (181). All other data from JANAF (51) who extrapolated 374 K to 631 K.

$(P_2O_5)_2(g)$

Dimeric Diphosphorus Pentoxide (ideal gas)

[Formation: $4P(c,l,1/4P_4(g)) + 5O_2(g) = (P_2O_5)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	45.126	96.525	96.525	0	-694.100	-638.113	467.744
300	45.325	96.805	96.525	.084	-694.125	-637.767	464.607
317.3	46.891	99.390	96.611	.882	-694.332	-634.507	437.030
317.3	46.891	99.390	96.611	.882	-694.960	-634.507	437.030
400	54.377	111.161	98.421	5.096	-695.767	-618.642	338.006
500	60.662	124.013	102.279	10.867	-696.167	-599.301	261.951
550	62.853	129.920	104.524	13.968	-696.199	-589.670	234.310
550	62.853	129.920	104.524	13.968	-707.831	-589.670	234.310
600	65.043	135.484	106.876	17.165	-707.468	-578.940	210.876
700	68.149	145.757	111.710	23.833	-706.578	-557.585	174.084
800	70.399	155.011	116.554	30.766	-705.547	-536.375	146.529
900	72.067	163.404	121.300	37.894	-704.417	-515.292	125.128
1000	73.329	171.066	125.900	45.166	-703.220	-494.344	108.037
1100	74.304	178.102	130.329	52.550	-701.979	-473.513	94.077
1200	75.069	184.602	134.585	60.020	-700.705	-452.802	82.465
1300	75.681	190.635	138.667	67.559	-699.406	-432.196	72.658
1400	76.175	196.263	142.583	75.152	-698.097	-411.693	64.267
1500	76.581	201.532	146.338	82.791	-696.776	-391.284	57.009
1600	76.918	206.486	149.945	90.466	-695.454	-370.960	50.670
1700	77.200	211.158	153.409	98.173	-694.129	-350.715	45.087
1800	77.439	215.577	156.741	105.905	-692.809	-330.546	40.133
1900	77.642	219.770	159.949	113.659	-691.501	-310.462	35.711
2000	77.817	223.757	163.041	121.433	-690.194	-290.440	31.737

Phase changes: 317.3 K, melting point of P; $\Delta H°$ = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H°$ = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 66.770 + 7.204\times10^{-3}T - 21.150\times10^{5}T^{-2}$

$H°- H°_{298} = 66.770\times10^{-3}T + 3.602\times10^{-6}T^{2} + 21.150\times10^{2}T^{-1} - 27.321$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -703.999 + 15.424\times10^{-3}T - 11.653\times10^{-6}T^{2} + 1889.000T^{-1}$

$\Delta Gf° = -703.999 - 15.424\times10^{-3}T\ln T + 11.653\times10^{-6}T^{2} + 944.500T^{-1} + 294.760\times10^{-3}T$

317.3-550 K: $\Delta Hf° = -702.745 + 5.452\times10^{-3}T + 1.087\times10^{-6}T^{2} + 1889.000T^{-1}$

$\Delta Gf° = -702.745 - 5.452\times10^{-3}T\ln T - 1.087\times10^{-6}T^{2} + 944.500T^{-1} + 237.415\times10^{-3}T$

550-2000 K: $\Delta Hf° = -716.586 + 10.804\times10^{-3}T + 1.071\times10^{-6}T^{2} + 1487.800T^{-1}$

$\Delta Gf° = -716.586 - 10.804\times10^{-3}T\ln T - 1.071\times10^{-6}T^{2} + 743.900T^{-1} + 297.006\times10^{-3}T$

Source: Data from JANAF (51). Enthalpy of formation based on P(white).

Pa(c,l)

Protactinium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15*	6.601	12.400	12.400	0
300	6.606	12.441	12.401	.012
400	6.903	14.382	12.662	.688
500	7.200	15.954	13.168	1.393
600	7.497	17.293	13.746	2.128
700	7.794	18.471	14.340	2.892
800	8.091	19.531	14.924	3.686
900	8.388	20.501	15.490	4.510
1000	8.685	21.401	16.037	5.364
1100	8.982	22.242	16.563	6.247
1200	9.279	23.037	17.070	7.160
1300	9.576	23.791	17.558	8.103
1400	9.873	24.511	18.028	9.076
1443	10.001	24.812	18.227	9.503
1443	9.500	25.912	18.227	11.090
1500	9.500	26.280	18.526	11.631
1600	9.500	26.893	19.030	12.581
1700	9.500	27.469	19.510	13.531
1800	9.500	28.012	19.967	14.481
1845	9.500	28.247	20.166	14.909
1845	11.300	29.845	20.166	17.859
1900	11.300	30.177	20.451	18.480
2000	11.300	30.757	20.952	19.610
2100	11.300	31.308	21.432	20.740
2200	11.300	31.834	21.893	21.870
2300	11.300	32.336	22.336	23.000
2400	11.300	32.817	22.763	24.130
2500	11.300	33.279	23.175	25.260

*All data estimated.

Phase changes: 1443 K, α - β transition of Pa; ΔH° = 1.587 kcal/mol.
1845 K, melting point of Pa; ΔH° = 2.950 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1443 K: $Cp^\circ = 5.711 + 2.974\times10^{-3}T + 0.003\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.711\times10^{-3}T + 1.487\times10^{-6}T^2 - 0.003\times10^{2}T^{-1} - 1.834$

1443-1845 K: $Cp^\circ = 9.500$

$H^\circ - H^\circ_{298} = 9.500\times10^{-3}T - 2.619$

1845-2500 K: $Cp^\circ = 11.300$

$H^\circ - H^\circ_{298} = 11.300\times10^{-3}T - 2.990$

Source: Data are those estimated by Oetting (167).

Pa(g)

Protactinium (ideal monatomic gas)

[Formation: Pa(c,l) = Pa(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.476	47.308	47.308	0	145.000	134.592	-98.657
300	5.482	47.342	47.309	.010	144.998	134.528	-98.002
400	5.813	48.966	47.528	.575	144.887	131.053	-71.603
500	6.084	50.293	47.951	1.171	144.778	127.608	-55.777
600	6.328	51.424	48.439	1.791	144.663	124.184	-45.234
700	6.564	52.417	48.937	2.436	144.544	120.782	-37.709
800	6.797	53.309	49.429	3.104	144.418	117.396	-32.071
900	7.022	54.123	49.906	3.795	144.285	114.025	-27.689
1000	7.233	54.874	50.366	4.508	144.144	110.671	-24.187
1100	7.427	55.572	50.807	5.241	143.994	107.331	-21.324
1200	7.603	56.226	51.232	5.993	143.833	104.006	-18.942
1300	7.762	56.841	51.640	6.761	143.658	100.693	-16.928
1400	7.905	57.422	52.033	7.545	143.469	97.394	-15.204
1443	7.960	57.662	52.197	7.886	143.383	95.981	-14.537
1443	7.960	57.662	52.197	7.886	141.796	95.981	-14.537
1500	8.034	57.971	52.410	8.342	141.711	94.174	-13.721
1600	8.153	58.494	52.775	9.151	141.570	91.008	-12.431
1700	8.262	58.991	53.125	9.972	141.441	87.854	-11.294
1800	8.364	59.467	53.465	10.803	141.322	84.703	-10.284
1845	8.407	59.674	53.614	11.180	141.271	83.288	-9.866
1845	8.407	59.674	53.614	11.180	138.321	83.288	-9.866
1900	8.459	59.921	53.793	11.644	138.164	81.650	-9.392
2000	8.548	60.357	54.109	12.495	137.885	78.685	-8.598
2100	8.632	60.777	54.418	13.354	137.614	75.729	-7.881
2200	8.712	61.180	54.716	14.221	137.351	72.790	-7.231
2300	8.788	61.569	55.006	15.096	137.096	69.860	-6.638
2400	8.859	61.945	55.287	15.979	136.849	66.942	-6.096
2500	8.927	62.308	55.561	16.868	136.608	64.036	-5.598

Phase changes: 1443 K, α - β transition point of Pa; $\Delta H° = 1.587$ kcal/mol.
1845 K, melting point of Pa; $\Delta H° = 2.950$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 5.603 + 1.566\times10^{-3}T - 0.528\times10^{5}T^{-2}$

$H°- H°_{298} = 5.603\times10^{-3}T + 0.783\times10^{-6}T^{2} + 0.528\times10^{2}T^{-1} - 1.917$

Formation equations (kcal/mol):

298.15-1443 K: $\Delta Hf° = 144.917 - 0.108\times10^{-3}T - 0.704\times10^{-6}T^{2} + 53.100T^{-1}$

$\Delta Gf° = 144.917 + 0.108\times10^{-3}T\ln T + 0.704\times10^{-6}T^{2} + 26.550T^{-1} - 35.752\times10^{-3}T$

1443-1845 K: $\Delta Hf° = 145.701 - 3.897\times10^{-3}T + 0.783\times10^{-6}T^{2} + 52.800T^{-1}$

$\Delta Gf° = 145.701 + 3.897\times10^{-3}T\ln T - 0.783\times10^{-6}T^{2} + 26.400T^{-1} - 61.713\times10^{-3}T$

1845-2500 K: $\Delta Hf° = 146.072 - 5.697\times10^{-3}T + 0.783\times10^{-6}T^{2} + 52.800T^{-1}$

$\Delta Gf° = 146.072 + 5.697\times10^{-3}T\ln T - 0.783\times10^{-6}T^{2} + 26.400T^{-1} - 75.451\times10^{-3}T$

Source: Data from Oetting (167).

Pb(c,l)

Lead

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.370	15.490	15.490	0
300	6.370	15.530	15.490	.012
400	6.530	17.380	15.742	.655
500	6.770	18.860	16.220	1.320
600	7.030	20.120	16.765	2.013
600.65	7.030	20.130	16.772	2.017
600.65	7.320	22.040	16.772	3.164
700	7.250	23.150	17.599	3.886
800	7.170	24.120	18.358	4.610
900	7.090	24.960	19.047	5.322
1000	7.020	25.700	19.672	6.028
1100	6.950	26.360	20.245	6.727
1200	6.880	26.970	20.789	7.417
1300	6.840	27.510	21.276	8.104
1400*	6.840	28.020	21.743	8.788
1500	6.840	28.490	22.175	9.472
1600	6.840	28.920	22.573	10.156
1700	6.840	29.350	22.974	10.840
1800	6.840	29.740	23.338	11.524
1900	6.840	30.110	23.685	12.208
2000	6.840	30.460	24.014	12.892

*Data above 1300 K extrapolated.

Phase changes: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.
2023 K, boiling point of Pb; ΔH° = 42.5 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600.65 K:

$$Cp^\circ = 4.851 + 3.528\times10^{-3}T + 0.414\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 4.851\times10^{-3}T + 1.764\times10^{-6}T^2 - 0.414\times10^{2}T^{-1} - 1.464$$

600.65-2000 K:

$$Cp^\circ = 7.415 - 0.426\times10^{-3}T + 0.580\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 7.415\times10^{-3}T - 0.213\times10^{-6}T^2 - 0.580\times10^{2}T^{-1} - 1.116$$

Sources: Entropy at 298 K from CODATA (36). All other data from Hultgren (99) who extrapolated above 1300 K by assuming constant heat capacity.

Pb(g)

Lead (ideal monatomic gas)

[Formation: Pb(c,l) = Pb(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	$C_p°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta H_f°$	$\Delta G_f°$	
298.15	4.968	41.890	41.890	0	46.750	38.879	-28.499
300	4.968	41.921	41.891	.009	46.747	38.830	-28.287
400	4.968	43.350	42.085	.506	46.601	36.213	-19.786
500	4.968	44.459	42.453	1.003	46.433	33.633	-14.701
600	4.968	45.365	42.865	1.500	46.237	31.090	-11.324
600.65	4.968	45.370	42.868	1.503	46.236	31.076	-11.307
600.65	4.968	45.370	42.868	1.503	45.089	31.076	-11.307
700	4.968	46.130	43.279	1.996	44.860	28.774	-8.984
800	4.969	46.794	43.678	2.493	44.633	26.494	-7.238
900	4.972	47.379	44.057	2.990	44.418	24.241	-5.886
1000	4.978	47.903	44.415	3.488	44.210	22.007	-4.810
1100	4.992	48.379	44.755	3.986	44.009	19.788	-3.931
1200	5.017	48.814	45.075	4.487	43.820	17.607	-3.207
1300	5.056	49.217	45.379	4.990	43.636	15.417	-2.592
1400	5.113	49.594	45.666	5.499	43.461	13.257	-2.070
1500	5.191	49.949	45.940	6.014	43.292	11.103	-1.618
1600	5.290	50.287	46.201	6.537	43.131	8.944	-1.222
1700	5.411	50.611	46.451	7.072	42.982	6.838	-.879
1800	5.554	50.924	46.691	7.620	42.846	4.715	-.572
1900	5.716	51.229	46.922	8.184	42.726	2.600	-.299
2000	5.899	51.527	47.145	8.764	42.622	.488	-.053

Phase change: 600.65 K, melting point of Pb; $\Delta H°$ = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p° = 4.626 + 0.408\times10^{-3}T + 0.196\times10^{5}T^{-2}$

$H°- H°_{298} = 4.626\times10^{-3}T + 0.204\times10^{-6}T^{2} - 0.196\times10^{2}T^{-1} - 1.332$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta H_f° = 46.883 - 0.225\times10^{-3}T - 1.560\times10^{-6}T^{2} + 21.800T^{-1}$

$\Delta G_f° = 46.883 + 0.225\times10^{-3}T\ln T + 1.560\times10^{-6}T^{2} + 10.900T^{-1} - 28.715\times10^{-3}T$

600.65-2000 K: $\Delta H_f° = 46.535 - 2.789\times10^{-3}T + 0.417\times10^{-6}T^{2} + 38.400T^{-1}$

$\Delta G_f° = 46.535 + 2.789\times10^{-3}T\ln T - 0.417\times10^{-6}T^{2} + 19.200T^{-1} - 43.376\times10^{-3}T$

Source: Data from JANAF (51).

$Pb_2(g)$

Lead (ideal diatomic gas)

[Formation: $2Pb(c,l) = Pb_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.825	67.216	67.216	0	79.500	68.696	-50.355
300	8.828	67.270	67.217	.016	79.492	68.629	-49.996
400	8.964	69.830	67.563	.907	79.097	65.069	-35.552
500	9.050	71.840	68.226	1.807	78.667	61.607	-26.928
600	9.115	73.496	68.969	2.716	78.190	58.236	-21.212
600.65	9.115	73.506	68.974	2.722	78.188	58.219	-21.183
600.65	9.115	73.506	68.974	2.722	75.894	58.219	-21.183
700	9.169	74.905	69.719	3.630	75.358	55.334	-17.276
800	9.219	76.133	70.447	4.549	74.829	52.515	-14.346
900	9.265	77.222	71.140	5.474	74.330	49.758	-12.083
1000	9.309	78.200	71.798	6.402	73.846	47.046	-10.282
1100	9.351	79.089	72.421	7.335	73.381	44.375	-8.816
1200	9.393	79.905	73.011	8.273	72.939	41.781	-7.609
1300	9.434	80.658	73.570	9.214	72.506	39.177	-6.586
1400	9.475	81.359	74.103	10.159	72.083	36.636	-5.719
1500	9.515	82.014	74.608	11.109	71.665	34.114	-4.970
1600	9.555	82.629	75.090	12.063	71.251	31.589	-4.315
1700	9.595	83.210	75.551	13.020	70.840	29.173	-3.750
1800	9.635	83.759	75.991	13.982	70.434	26.732	-3.246
1900	9.674	84.281	76.414	14.947	70.031	24.315	-2.797
2000	9.714	84.779	76.821	15.916	69.632	21.914	-2.395

Phase change: 600.65 melting point of Pb; $\Delta H° = 1.147$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.931 + 0.396\times10^{-3}T - 0.200\times10^{5}T^{-2}$

$H°- H°_{298} = 8.931\times10^{-3}T + 0.198\times10^{-6}T^{2} + 0.200\times10^{2}T^{-1} - 2.747$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf° = 79.681 - 0.771\times10^{-3}T - 3.330\times10^{-6}T^{2} + 102.800T^{-1}$

$\Delta Gf° = 79.681 + 0.771\times10^{-3}T\ln T + 3.330\times10^{-6}T^{2} + 51.400T^{-1} - 42.807\times10^{-3}T$

600.65-2000 K: $\Delta Hf° = 78.985 - 5.899\times10^{-3}T + 0.624\times10^{-6}T^{2} + 136.000T^{-1}$

$\Delta Gf° = 78.985 + 5.899\times10^{-3}T\ln T - 0.624\times10^{-6}T^{2} + 68.000T^{-1} - 72.129\times10^{-3}T$

Source: Data from JANAF (51).

PbO(red,yellow,l)

Lead Oxide, Litharge

[Formation: $Pb(c,l) + 0.5O_2(g) = PbO(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.950	15.900	15.900	0	-52.340	-45.157	33.100
300	10.965	15.968	15.901	.020	-52.339	-45.113	32.864
400	11.570	19.205	16.337	1.147	-52.209	-42.721	23.342
500	12.049	21.840	17.182	2.329	-52.058	-40.368	17.645
600	12.463	24.074	18.149	3.555	-51.903	-38.046	13.858
600.65	12.465	24.087	18.155	3.563	-51.901	-38.029	13.837
600.65	12.465	24.087	18.155	3.563	-53.048	-38.029	13.837
700	12.846	26.024	19.138	4.820	-52.900	-35.558	11.101
762	13.075	27.128	19.746	5.625	-52.792	-34.026	9.759
762	13.006	27.653	19.746	6.025	-52.392	-34.026	9.759
800	13.129	28.289	20.138	6.521	-52.321	-33.113	9.046
900	13.445	29.854	21.132	7.850	-52.112	-30.723	7.460
1000	13.754	31.286	22.076	9.210	-51.871	-28.362	6.198
1100	14.058	32.611	22.974	10.601	-51.599	-26.030	5.172
1159	14.236	33.350	23.484	11.435	-51.421	-24.653	4.649
1159	13.836	38.639	23.484	17.565	-45.291	-24.653	4.649
1200	13.836	39.120	24.010	18.132	-45.181	-23.925	4.357
1300	13.836	40.227	25.215	19.516	-44.913	-22.176	3.728
1400	13.836	41.253	26.325	20.899	-44.646	-20.435	3.190
1500	13.836	42.207	27.352	22.283	-44.381	-18.716	2.727

Phase changes: 600.65 K, melting point of Pb; $\Delta H° = 1.147$ kcal/mol.
762 K, red-yellow transition of PbO; $\Delta H° = 0.400$ kcal/mol.
1159 K, melting point of PbO; $\Delta H° = 6.130$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-762 K: $Cp° = 10.416 + 3.634\times10^{-3}T - 0.488\times10^{5}T^{-2}$

$H°- H°_{298} = 10.416\times10^{-3}T + 1.817\times10^{-6}T^{2} + 0.488\times10^{2}T^{-1} - 3.431$

762-1159 K: $Cp° = 10.804 + 2.994\times10^{-3}T - 0.458\times10^{5}T^{-2}$

$H°- H°_{298} = 10.804\times10^{-3}T + 1.497\times10^{-6}T^{2} + 0.458\times10^{2}T^{-1} - 3.137$

1159-1500 K: $Cp° = 13.836$

$H°- H°_{298} = 13.836\times10^{-3}T + 1.529$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf° = -53.130 + 1.950\times10^{-3}T - 0.199\times10^{-6}T^{2} + 67.600T^{-1}$

$\Delta Gf° = -53.130 - 1.950\times10^{-3}T\ln T + 0.199\times10^{-6}T^{2} + 33.800T^{-1} + 37.415\times10^{-3}T$

600.65-762 K: $\Delta Hf° = -53.478 - 0.614\times10^{-3}T + 1.779\times10^{-6}T^{2} + 84.200T^{-1}$

$\Delta Gf° = -53.478 + 0.614\times10^{-3}T\ln T - 1.779\times10^{-6}T^{2} + 42.100T^{-1} + 22.754\times10^{-3}T$

762-1159 K: $\Delta Hf° = -53.184 - 0.226\times10^{-3}T + 1.459\times10^{-6}T^{2} + 81.200T^{-1}$

$\Delta Gf° = -53.184 + 0.226\times10^{-3}T\ln T - 1.459\times10^{-6}T^{2} + 40.600T^{-1} + 24.701\times10^{-3}T$

1159-1500 K: $\Delta Hf° = -48.518 + 2.806\times10^{-3}T - 0.038\times10^{-6}T^{2} + 35.400T^{-1}$

$\Delta Gf° = -48.518 - 2.806\times10^{-3}T\ln T + 0.038\times10^{-6}T^{2} + 17.700T^{-1} + 40.349\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (236). Low-temperature heat capacities from King (128). High-temperature data based on: red PbO, Spencer (209); yellow PbO and enthalpy of fusion Rodigina (189); and heat capacity of liquid, Knacke (136).

PbO(yellow,l)

Lead Oxide, Massicot

[Formation: $Pb(c,l) + 0.5O_2(g) = PbO(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.950	16.420	16.420	0	-51.940	-44.912	32.921
300	10.966	16.488	16.421	.020	-51.938	-44.869	32.686
400	11.607	19.735	16.860	1.150	-51.806	-42.530	23.237
500	12.070	22.376	17.706	2.335	-51.652	-40.230	17.584
600	12.454	24.612	18.675	3.562	-51.495	-37.962	13.827
600.65	12.456	24.625	18.682	3.570	-51.494	-37.945	13.806
600.65	12.456	24.625	18.682	3.570	-52.641	-37.945	13.806
700	12.801	26.558	19.665	4.825	-52.494	-35.526	11.092
800*	13.129	28.289	20.638	6.121	-52.321	-33.113	9.046
900	13.445	29.854	21.576	7.450	-52.111	-30.723	7.460
1000	13.754	31.286	22.476	8.810	-51.871	-28.362	6.198
1100	14.058	32.611	23.337	10.201	-51.598	-26.030	5.172
1159	14.236	33.350	23.829	11.035	-51.421	-24.653	4.649
1159	13.836	38.639	23.829	17.165	-45.291	-24.653	4.649
1200	13.836	39.120	24.343	17.732	-45.181	-23.925	4.357
1300	13.836	40.227	25.522	19.116	-44.913	-22.176	3.728
1400	13.836	41.253	26.611	20.499	-44.646	-20.435	3.190
1500	13.836	42.207	27.618	21.883	-44.381	-18.716	2.727

*Yellow PbO is metastable below 762 K.

Phase changes: 600.65 K, melting point of Pb; $\Delta H° = 1.147$ kcal/mol.
1159 K, melting point of PbO; $\Delta H° = 6.130$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1159 K:

$$Cp° = 10.882 + 2.944\times10^{-3}T - 0.720\times10^{5}T^{-2}$$

$$H°- H°_{298} = 10.882\times10^{-3}T + 1.472\times10^{-6}T^{2} + 0.720\times10^{2}T^{-1} - 3.617$$

1159-1500 K:

$$Cp° = 13.836$$

$$H°- H°_{298} = 13.836\times10^{-3}T + 1.129$$

Formation equations (kcal/mol):

298.15-600.65 K:

$$\Delta Hf° = -52.917 + 2.416\times10^{-3}T - 0.544\times10^{-6}T^{2} + 90.800T^{-1}$$

$$\Delta Gf° = -52.917 - 2.416\times10^{-3}T\ln T + 0.544\times10^{-6}T^{2} + 45.400T^{-1} + 39.941\times10^{-3}T$$

600.65-1159 K:

$$\Delta Hf° = -53.264 - 0.148\times10^{-3}T + 1.434\times10^{-6}T^{2} + 107.400T^{-1}$$

$$\Delta Gf° = -53.264 + 0.148\times10^{-3}T\ln T - 1.434\times10^{-6}T^{2} + 53.700T^{-1} + 25.280\times10^{-3}T$$

1159-1500 K:

$$\Delta Hf° = -48.519 + 2.806\times10^{-3}T - 0.038\times10^{-6}T^{2} + 35.400T^{-1}$$

$$\Delta Gf° = -48.519 - 2.806\times10^{-3}T\ln T + 0.038\times10^{-6}T^{2} + 17.700T^{-1} + 40.347\times10^{-3}T$$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (236). Low-temperature heat capacities from King (128). High-temperature data based on: yellow PbO and enthalpy of fusion, Rodigina (189) and heat capacity of liquid, Knacke (136).

PbO(g)

Lead Oxide (ideal gas)

[Formation: $Pb(c,l) + 0.5O_2(g) = PbO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.770	57.343	57.343	0	16.800	11.627	-8.523
300	7.778	57.392	57.345	.014	16.795	11.594	-8.446
400	8.155	59.685	57.655	.812	16.595	9.891	-5.404
500	8.401	61.533	58.251	1.641	16.394	8.238	-3.601
600	8.562	63.080	58.930	2.490	16.172	6.626	-2.413
600.65	8.563	63.089	58.934	2.496	16.172	6.618	-2.408
600.65	8.563	63.089	58.934	2.496	15.025	6.618	-2.408
700	8.671	64.408	59.619	3.352	14.772	5.246	-1.638
800	8.750	65.571	60.292	4.223	14.520	3.904	-1.066
900	8.808	66.605	60.937	5.101	14.279	2.593	-.630
1000	8.853	67.536	61.552	5.984	14.043	1.302	-.285
1100	8.889	68.381	62.135	6.871	13.811	.033	-.007
1200	8.918	69.156	62.688	7.762	13.589	-1.198	.218
1300	8.943	69.871	63.213	8.655	13.366	-2.434	.409
1400	8.965	70.534	63.713	9.550	13.146	-3.637	.568
1500	8.984	71.154	64.189	10.448	12.924	-4.832	.704
1600	9.001	71.734	64.642	11.347	12.701	-6.026	.823
1700	9.017	72.280	65.075	12.248	12.477	-7.163	.921
1800	9.031	72.796	65.490	13.150	12.251	-8.314	1.009
1900	9.045	73.285	65.888	14.054	12.024	-9.451	1.087
2000	9.058	73.749	66.270	14.959	11.795	-10.577	1.156

Phase change: 600.65 K, melting point of Pb; $\Delta H° = 1.147$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.646 + 0.252\times10^{-3}T - 0.846\times10^{5}T^{-2}$

$H°- H°_{298} = 8.646\times10^{-3}T + 0.126\times10^{-6}T^{2} + 0.846\times10^{2}T^{-1} - 2.873$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf° = 16.567 + 0.180\times10^{-3}T - 1.890\times10^{-6}T^{2} + 103.400T^{-1}$

$\Delta Gf° = 16.567 - 0.180\times10^{-3}T\ln T + 1.890\times10^{-6}T^{2} + 51.700T^{-1} - 16.690\times10^{-3}T$

600.65-2000 K: $\Delta Hf° = 16.220 - 2.384\times10^{-3}T + 0.088\times10^{-6}T^{2} + 120.000T^{-1}$

$\Delta Gf° = 16.220 + 2.384\times10^{-3}T\ln T - 0.088\times10^{-6}T^{2} + 60.000T^{-1} - 31.351\times10^{-3}T$

Source: Data from Chase (31).

$PbO_2(c)$

Lead Dioxide

[Formation: $Pb(c,l) + O_2(g) = PbO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.580	17.156	17.156	0	-66.300	-52.186	38.253
300*	14.608	17.246	17.156	.027	-66.298	-52.098	37.953
400	15.793	21.618	17.743	1.550	-66.128	-47.387	25.891
500	16.705	25.244	18.892	3.176	-65.898	-42.730	18.677
600	17.499	28.361	20.216	4.887	-65.635	-38.121	13.886
600.65	17.504	28.380	20.225	4.898	-65.633	-38.090	13.859
600.65	17.504	28.380	20.225	4.898	-66.780	-38.090	13.859
700	18.237	31.114	21.580	6.674	-66.499	-33.367	10.417

*Data above 298 K estimated.

Phase change: 600.65 K, melting point of Pb; $\Delta H° = 1.147$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 13.635 + 6.932\times10^{-3}T - 0.997\times10^{5}T^{-2}$

$H°- H°_{298} = 13.635\times10^{-3}T + 3.466\times10^{-6}T^{2} + 0.997\times10^{2}T^{-1} - 4.708$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf° = -67.192 + 1.554\times10^{-3}T + 1.199\times10^{-6}T^{2} + 95.900T^{-1}$

$\Delta Gf° = -67.192 - 1.554\times10^{-3}T\ln T - 1.199\times10^{-6}T^{2} + 47.950T^{-1} + 59.001\times10^{-3}T$

600.65-700 K: $\Delta Hf° = -67.539 - 1.010\times10^{-3}T + 3.176\times10^{-6}T^{2} + 112.500T^{-1}$

$\Delta Gf° = -67.539 + 1.010\times10^{-3}T\ln T - 3.176\times10^{-6}T^{2} + 56.250T^{-1} + 44.340\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities and entropy at 298 K from Duisman (57). High-temperature data estimated.

$Pb_3O_4(c)$

Trilead Tetroxide, Minium

[Formation: $3Pb(c,l) + 2O_2(g) = Pb_3O_4(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	37.030	50.660	50.660	0	-171.770	-143.798	105.405
300	37.128	50.889	50.660	.069	-171.763	-143.623	104.628
400	41.360	62.188	52.173	4.006	-171.175	-134.322	73.389
500	44.000	71.720	55.154	8.283	-170.355	-125.204	54.726
600	45.600	79.893	58.613	12.768	-169.459	-116.262	42.348
600.65	45.606	79.942	58.636	12.798	-169.451	-116.199	42.279
600.65	45.606	79.942	58.636	12.798	-172.892	-116.199	42.279
700	46.600	86.997	62.171	17.378	-172.024	-106.892	33.373
800	47.600	93.285	65.675	22.088	-171.082	-97.646	26.675
900	48.600	98.949	69.062	26.898	-170.036	-88.524	21.496
1000	49.600	104.122	72.314	31.808	-168.898	-79.540	17.383

Phase change: 600.65 K, melting point of Pb; $\Delta H° = 1.147$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 42.741 + 7.680\times10^{-3}T - 7.113\times10^{5}T^{-2}$

$H°- H°_{298} = 42.741\times10^{-3}T + 3.840\times10^{-6}T^{2} + 7.113\times10^{2}T^{-1} - 15.470$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf° = -178.144 + 13.728\times10^{-3}T - 2.458\times10^{-6}T^{2} + 745.100T^{-1}$

$\Delta Gf° = -178.144 - 13.728\times10^{-3}T\ln T + 2.458\times10^{-6}T^{2} + 372.550T^{-1} + 188.490\times10^{-3}T$

600.65-1000 K: $\Delta Hf° = -179.187 + 6.036\times10^{-3}T + 3.473\times10^{-6}T^{2} + 794.900T^{-1}$

$\Delta Gf° = -179.187 - 6.036\times10^{-3}T\ln T - 3.473\times10^{-6}T^{2} + 397.450T^{-1} + 144.507\times10^{-3}T$

Source: Data from Chase (31).

Pd(c,l)

Palladium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.188	9.013	9.013	0
300	6.193	9.051	9.014	.011
400	6.359	10.855	9.257	.639
500	6.507	12.290	9.726	1.282
600	6.643	13.488	10.255	1.940
700	6.774	14.522	10.792	2.611
800	6.903	15.435	11.316	3.295
900	7.032	16.256	11.822	3.991
1000	7.161	17.003	12.302	4.701
1100	7.291	17.692	12.762	5.423
1200	7.421	18.332	13.200	6.159
1300	7.553	18.931	13.617	6.908
1400	7.686	19.496	14.017	7.670
1500	7.820	20.030	14.400	8.445
1600	7.956	20.539	14.768	9.234
1700	8.093	21.026	15.122	10.036
1800	8.231	21.492	15.463	10.852
1827	8.269	21.615	15.553	11.075
1827	9.060	23.788	15.553	15.045
1900	9.060	24.143	15.877	15.706
2000	9.060	24.608	16.302	16.612
2100	9.060	25.050	16.708	17.518
2200	9.060	25.471	17.096	18.424
2300	9.060	25.874	17.470	19.330
2400	9.060	26.260	17.828	20.236
2500	9.060	26.629	18.172	21.142

Phase changes: 1827 K, melting point of Pd; ΔH° = 3.970 kcal/mol.
3237 K, boiling point of Pd; ΔH° = 85.4 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1827 K: $Cp^\circ = 5.872 + 1.302\times10^{-3}T - 0.065\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.872\times10^{-3}T + 0.651\times10^{-6}T^2 + 0.065\times10^{2}T^{-1} - 1.830$

1827-2500 K: $Cp^\circ = 9.060$

$H^\circ - H^\circ_{298} = 9.060\times10^{-3}T - 1.508$

Sources: Low-temperature heat capacities and entropy at 298 K from Furukawa (72). Data for Pd(c) based on Jaeger (101) and data for Pd(l) based on Treverton (225).

Pd(g)

Palladium (ideal monatomic gas)

[Formation: Pd(c,l) = Pd(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	4.968	39.902	39.902	0	90.400	81.190	-59.513
300	4.968	39.933	39.903	.009	90.398	81.133	-59.105
400	4.968	41.362	40.097	.506	90.267	78.064	-42.652
500	4.968	42.471	40.465	1.003	90.121	75.031	-32.795
600	4.969	43.376	40.876	1.500	89.960	72.027	-26.236
700	4.972	44.143	41.290	1.997	89.786	69.051	-21.559
800	4.984	44.807	41.689	2.494	89.599	66.101	-18.058
900	5.017	45.396	42.069	2.994	89.403	63.177	-15.341
1000	5.084	45.928	42.429	3.499	89.198	60.273	-13.172
1100	5.201	46.417	42.769	4.013	88.990	57.393	-11.403
1200	5.380	46.877	43.093	4.541	88.782	54.528	-9.931
1300	5.625	47.317	43.401	5.091	88.583	51.681	-8.688
1400	5.939	47.745	43.696	5.668	88.398	48.849	-7.626
1500	6.315	48.167	43.980	6.281	88.236	46.031	-6.707
1600	6.743	48.588	44.255	6.933	88.099	43.221	-5.904
1700	7.206	49.011	44.523	7.630	87.994	40.419	-5.196
1800	7.688	49.436	44.783	8.375	87.923	37.624	-4.568
1827	7.818	49.551	44.853	8.584	87.909	36.869	-4.410
1827	7.818	49.551	44.853	8.584	83.939	36.869	-4.410
1900	8.169	49.865	45.040	9.168	83.862	34.990	-4.025
2000	8.632	50.295	45.291	10.008	83.796	32.422	-3.543
2100	9.060	50.727	45.540	10.893	83.775	29.853	-3.107
2200	9.442	51.158	45.786	11.819	83.795	27.284	-2.710
2300	9.768	51.585	46.028	12.780	83.850	24.715	-2.348
2400	10.033	52.006	46.269	13.770	83.934	22.144	-2.016
2500	10.235	52.420	46.506	14.784	84.042	19.565	-1.710

Phase change: 1827 K, melting point of Pd; ΔH° = 3.970 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp^\circ = 2.628 + 2.704\times10^{-3}T + 1.363\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 2.628\times10^{-3}T + 1.352\times10^{-6}T^2 - 1.363\times10^{2}T^{-1} - 0.447$

Formation equations (kcal/mol):

298.15-1827 K: $\Delta Hf^\circ = 91.784 - 3.244\times10^{-3}T + 0.701\times10^{-6}T^2 - 142.800T^{-1}$

$\Delta Gf^\circ = 91.784 + 3.244\times10^{-3}T\ln T - 0.701\times10^{-6}T^2 - 71.400T^{-1} - 53.001\times10^{-3}T$

1827-2500 K: $\Delta Hf^\circ = 91.462 - 6.432\times10^{-3}T + 1.352\times10^{-6}T^2 - 136.300T^{-1}$

$\Delta Gf^\circ = 91.462 + 6.432\times10^{-3}T\ln T - 1.352\times10^{-6}T^2 - 68.150T^{-1} - 75.580\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). All other data from Hilsenrath (94).

Pr(c,l)

Praseodymium

T, K	cal/mol·K			$H°- H^{\circ}_{298}$, kcal/mol
	Cp°	S°	$-(G°- H^{\circ}_{298})/T$	
298.15	6.560	17.670	17.670	0
300	6.560	17.710	17.670	.012
400	6.790	19.630	17.932	.679
500	7.100	21.180	18.434	1.373
600	7.530	22.500	18.995	2.103
700	8.000	23.700	19.584	2.881
800	8.500	24.800	20.169	3.705
900	9.040	25.840	20.749	4.582
1000	9.650	26.820	21.306	5.514
1068	10.010	27.460	21.672	6.183
1068	9.190	28.170	21.672	6.940
1100	9.190	28.440	21.864	7.234
1200	9.190	29.240	22.446	8.153
1204	9.190	29.280	22.474	8.190
1204	10.270	30.640	22.474	9.836
1300	10.270	31.430	23.105	10.822
1400	10.270	32.190	23.726	11.849
1500*	10.270	32.900	24.316	12.876
1600	10.270	33.560	24.870	13.904
1700	10.270	34.190	25.407	14.931
1800	10.270	34.770	25.904	15.958
1900	10.270	35.330	26.391	16.985
2000	10.270	35.860	26.854	18.012

*Data above 1400 K extrapolated.

Phase changes: 1068 K, α - β transition of Pr; $\Delta H°$ = 0.757 kcal/mol.
1204 K, melting point of Pr; $\Delta H°$ = 1.646 kcal/mol.
3785 K, boiling point of Pr; $\Delta H°$ = 70.9 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1068 K: $Cp° = 4.170 + 5.326\times10^{-3}T + 0.713\times10^{5}T^{-2}$

$H°- H^{\circ}_{298} = 4.170\times10^{-3}T + 2.663\times10^{-6}T^{2} - 0.713\times10^{2}T^{-1} - 1.241$

1068-1204 K: $Cp° = 9.190$

$H°- H^{\circ}_{298} = 9.190\times10^{-3}T - 2.875$

1204-2000 K: $Cp° = 10.270$

$H°- H^{\circ}_{298} = 10.270\times10^{-3}T - 2.529$

Source: Data from Hultgren (99) who extrapolated above 1400 K by assuming constant heat capacity.

Pr(g)

Praseodymium (ideal monatomic gas)

[Formation: Pr(c,l) = Pr(g)]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.105	45.339	45.339	0	85.000	76.750	-56.259
300	5.109	45.370	45.340	.009	84.997	76.699	-55.874
400	5.385	46.876	45.543	.533	84.854	73.956	-40.407
500	5.701	48.111	45.935	1.088	84.715	71.249	-31.143
600	5.987	49.177	46.389	1.673	84.570	68.564	-24.974
700	6.225	50.118	46.855	2.284	84.403	65.910	-20.578
800	6.413	50.962	47.317	2.916	84.211	63.281	-17.287
900	6.558	51.726	47.765	3.565	83.983	60.686	-14.736
1000	6.662	52.423	48.197	4.226	83.712	58.109	-12.700
1068	6.710	52.863	48.480	4.681	83.498	56.369	-11.535
1068	6.710	52.863	48.480	4.681	82.741	56.369	-11.535
1100	6.732	53.061	48.610	4.896	82.662	55.579	-11.042
1200	6.771	53.649	49.007	5.571	82.418	53.127	-9.676
1204	6.772	53.672	49.022	5.598	82.408	53.036	-9.627
1204	6.772	53.672	49.022	5.598	80.762	53.036	-9.627
1300	6.787	54.192	49.385	6.249	80.427	50.836	-8.546
1400	6.783	54.695	49.746	6.928	80.079	48.572	-7.582
1500	6.766	55.162	50.091	7.606	79.730	46.337	-6.751
1600	6.739	55.598	50.422	8.281	79.377	44.116	-6.026
1700	6.707	56.005	50.739	8.953	79.022	41.936	-5.391
1800	6.671	56.388	51.042	9.622	78.664	39.752	-4.826
1900	6.634	56.747	51.333	10.287	78.302	37.610	-4.326
2000	6.598	57.087	51.613	10.949	77.937	35.483	-3.877

Phase changes: 1068 K, α - β transition point of Pr; $\Delta H° = 0.757$ kcal/mol.
1204 K, melting point of Pr; $\Delta H° = 1.646$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 5.955 + 0.570\times10^{-3}T - 0.907\times10^{5}T^{-2}$

$H°- H°_{298} = 5.955\times10^{-3}T + 0.285\times10^{-6}T^{2} + 0.907\times10^{2}T^{-1} - 2.105$

Formation equations (kcal/mol):

298.15-1068 K: $\Delta Hf° = 84.136 + 1.785\times10^{-3}T - 2.378\times10^{-6}T^{2} + 162.000T^{-1}$

$\Delta Gf° = 84.136 - 1.785\times10^{-3}T\ln T + 2.378\times10^{-6}T^{2} + 81.000T^{-1} - 16.221\times10^{-3}T$

1068-1204 K: $\Delta Hf° = 85.769 - 3.235\times10^{-3}T + 0.285\times10^{-6}T^{2} + 90.700T^{-1}$

$\Delta Gf° = 85.769 + 3.235\times10^{-3}T\ln T - 0.285\times10^{-6}T^{2} + 45.350T^{-1} - 49.882\times10^{-3}T$

1204-2000 K: $\Delta Hf° = 85.424 - 4.315\times10^{-3}T + 0.285\times10^{-6}T^{2} + 90.700T^{-1}$

$\Delta Gf° = 85.424 + 4.315\times10^{-3}T\ln T - 0.285\times10^{-6}T^{2} + 45.350T^{-1} - 57.256\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). All other data from Feber (58).

$PrO_{1.833}(c)$

Praseodymium Oxide

[Formation: $Pr(c) + 0.9165O_2(g) = PrO_{1.833}(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.200	19.100	19.100	0	-255.520	-242.556	177.796
300	15.213	19.194	19.101	.028	-255.516	-242.475	176.641
400	16.985	23.836	19.721	1.646	-255.216	-238.168	130.128
500	18.204	27.763	20.947	3.408	-254.818	-233.950	102.258
600	19.212	31.173	22.373	5.280	-254.368	-229.823	83.712
700	20.119	34.204	23.851	7.247	-253.892	-225.769	70.487
760	20.637	35.879	24.734	8.470	-253.594	-223.372	64.233
760	20.833	36.380	24.734	8.850	-253.214	-223.372	64.233
800	21.314	37.461	25.345	9.693	-253.001	-221.807	60.594
900	22.518	40.041	26.835	11.885	-252.432	-217.933	52.921
1000	23.721	42.475	28.278	14.197	-251.810	-214.134	46.798
1068	24.540	44.063	29.234	15.838	-251.360	-211.594	43.299
1068	24.540	44.063	29.234	15.838	-252.117	-211.594	43.299
1100	24.925	44.793	29.676	16.629	-251.867	-210.384	41.799

*Entropy and heat capacity at 298 K estimated.

Phase changes: 760 K, α - β transition point of $PrO_{1.833}$; $\Delta H° = 0.380$ kcal/mol.
1068 K, α - β transition point of Pr; $\Delta H° = 0.757$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-760 K:
$$Cp° = 15.176 + 7.654\times10^{-3}T - 2.007\times10^{5}T^{-2}$$
$$H°- H°_{298} = 15.176\times10^{-3}T + 3.827\times10^{-6}T^{2} + 2.007\times10^{2}T^{-1} - 5.538$$

760-1100 K:
$$Cp° = 11.919 + 11.856\times10^{-3}T - 0.562\times10^{5}T^{-2}$$
$$H°- H°_{298} = 11.919\times10^{-3}T + 5.928\times10^{-6}T^{2} + 0.562\times10^{2}T^{-1} - 3.706$$

Formation equations (kcal/mol):

298.15-760 K:
$$\Delta Hf° = -257.662 + 4.380\times10^{-3}T + 0.703\times10^{-6}T^{2} + 230.574T^{-1}$$
$$\Delta Gf° = -257.662 - 4.380\times10^{-3}T\ln T - 0.703\times10^{-6}T^{2} + 115.287T^{-1} + 74.533\times10^{-3}T$$

760-1068 K:
$$\Delta Hf° = -255.830 + 1.123\times10^{-3}T + 2.804\times10^{-6}T^{2} + 86.074T^{-1}$$
$$\Delta Gf° = -255.830 - 1.123\times10^{-3}T\ln T - 2.804\times10^{-6}T^{2} + 43.037T^{-1} + 52.239\times10^{-3}T$$

1068-1100 K:
$$\Delta Hf° = -254.196 - 3.897\times10^{-3}T + 5.467\times10^{-6}T^{2} + 14.774T^{-1}$$
$$\Delta Gf° = -254.196 + 3.897\times10^{-3}T\ln T - 5.467\times10^{-6}T^{2} + 7.387T^{-1} + 18.578\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Fitzgibbon (64). Entropy at 298 K estimated by Westrum (246). Heat capacity at 298 K estimated. High-temperature data based on Pankratz (174).

$Pr_2O_3(c)$

Dipraseodymium Trioxide, Praseodymium Sesquioxide

[Formation: $2Pr(c,1) + 1.5O_2(g) = Pr_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	28.200	37.200	37.200	0	-432.520	-411.158	301.383
300	28.244	37.375	37.202	.052	-432.511	-411.026	299.428
400	30.010	45.765	38.333	2.973	-431.990	-403.938	220.698
500	31.175	52.593	40.523	6.035	-431.412	-396.988	173.521
600	32.096	58.361	43.028	9.200	-430.839	-390.169	142.117
700	32.897	63.370	45.584	12.450	-430.312	-383.431	119.711
800	33.630	67.811	48.090	15.777	-429.830	-376.767	102.927
900	34.320	71.812	50.506	19.175	-429.408	-370.146	89.882
1000	34.982	75.463	52.823	22.640	-429.047	-363.585	79.460
1068	35.419	77.778	54.338	25.034	-428.845	-359.152	73.494
1068	35.419	77.778	54.338	25.034	-430.359	-359.152	73.494
1100	35.625	78.827	55.035	26.171	-430.215	-357.023	70.933
1200	36.254	81.954	57.150	29.765	-429.730	-350.389	63.814
1204	36.279	82.075	57.232	29.910	-429.711	-350.110	63.551
1204	36.279	82.075	57.232	29.910	-433.003	-350.110	63.551
1300	36.873	84.880	59.172	33.421	-432.697	-343.517	57.750
1400	37.487	87.635	61.107	37.139	-432.328	-336.674	52.557
1500	38.096	90.242	62.963	40.919	-431.908	-329.851	48.059
1600	38.704	92.721	64.747	44.759	-431.439	-323.075	44.129
1700	39.313	95.085	66.462	48.659	-430.916	-316.292	40.662
1800	39.925	97.350	68.116	52.621	-430.340	-309.591	37.589

*Heat capacity at 298 K estimated.

Phase changes: 1068 K, α - β transition point of Pr; $\Delta H° = 0.757$ kcal/mol.
1204 K, melting point of Pr; $\Delta H° = 1.646$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 29.134 + 6.066\times10^{-3}T - 2.439\times10^{5}T^{-2}$

$H°- H°_{298} = 29.134\times10^{-3}T + 3.033\times10^{-6}T^{2} + 2.439\times10^{2}T^{-1} - 9.774$

Formation equations (kcal/mol):

298.15-1068 K: $\Delta Hf° = -436.284 + 9.949\times10^{-3}T - 3.048\times10^{-6}T^{2} + 318.700T^{-1}$

$\Delta Gf° = -436.284 - 9.949\times10^{-3}T\ln T + 3.048\times10^{-6}T^{2} + 159.350T^{-1} + 138.257\times10^{-3}T$

1068-1204 K: $\Delta Hf° = -433.017 - 0.091\times10^{-3}T + 2.279\times10^{-6}T^{2} + 176.100T^{-1}$

$\Delta Gf° = -433.017 + 0.091\times10^{-3}T\ln T - 2.279\times10^{-6}T^{2} + 88.050T^{-1} + 70.934\times10^{-3}T$

1204-1800 K: $\Delta Hf° = -433.708 - 2.251\times10^{-3}T + 2.279\times10^{-6}T^{2} + 176.100T^{-1}$

$\Delta Gf° = -433.708 + 2.251\times10^{-3}T\ln T - 2.279\times10^{-6}T^{2} + 88.050T^{-1} + 56.187\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Fitzgibbon (64). Entropy at 298 K from Vasil'eva (232). Heat capacity at 298 K estimated. High-temperature data based on Pankratz (174).

Pt(c,1)

Platinum

T, K	cal/mol•K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.180	9.950	9.950	0
300	6.180	9.988	9.951	.011
400	6.330	11.789	10.194	.638
500	6.450	13.214	10.662	1.276
600	6.580	14.401	11.188	1.928
700	6.700	15.425	11.722	2.592
800	6.830	16.328	12.242	3.269
900	6.960	17.140	12.742	3.958
1000	7.080	17.879	13.220	4.659
1100	7.210	18.559	13.674	5.373
1200	7.330	19.192	14.109	6.100
1300	7.470	19.784	14.522	6.841
1400	7.590	20.342	14.918	7.593
1500	7.710	20.870	15.298	8.358
1600	7.840	21.371	15.662	9.135
1700	7.960	21.851	16.012	9.926
1800	8.090	22.309	16.348	10.729
1900	8.220	22.750	16.674	11.545
2000	8.340	23.175	16.989	12.372
2042	8.370	23.349	17.118	12.725
2042*	8.300	25.649	17.118	17.421
2100	8.300	25.881	17.356	17.902
2200	8.300	26.268	17.753	18.733

*Enthalpy and entropy of fusion, and heat capacity for Pt(l) estimated.

Phase change: 2042 K, melting point of Pt; ΔH° = 4.696 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2042 K: $Cp^\circ = 5.826 + 1.260\times10^{-3}T - 0.020\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.826\times10^{-3}T + 0.630\times10^{-6}T^2 + 0.020\times10^{2}T^{-1} - 1.800$

2042-2200 K: $Cp^\circ = 8.300$

$H^\circ - H^\circ_{298} = 8.300\times10^{-3}T + 0.472$

Sources: Entropy at 298 K from Wagman (237). All other data from Hultgren (99) who estimated entropy of fusion and heat capacity for Pt(l).

Pt(g)

Platinum (ideal monatomic gas)

[Formation: Pt(c,1) = Pt(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH_f°	ΔG_f°	
298.15	6.102	45.960	45.960	0	135.100	124.364	-91.160
300	6.113	45.998	45.961	.011	135.100	124.297	-90.549
400	6.459	47.815	46.205	.644	135.106	120.696	-65.944
500	6.435	49.259	46.679	1.290	135.114	117.091	-51.180
600	6.260	50.417	47.207	1.926	135.098	113.488	-41.338
700	6.059	51.367	47.736	2.542	135.050	109.891	-34.309
800	5.877	52.164	48.242	3.138	134.969	106.300	-29.039
900	5.728	52.847	48.716	3.718	134.860	102.724	-24.944
1000	5.609	53.444	49.159	4.285	134.726	99.161	-21.671
1100	5.517	53.974	49.573	4.841	134.568	95.612	-18.996
1200	5.447	54.451	49.960	5.389	134.389	92.078	-16.770
1300	5.395	54.885	50.323	5.931	134.190	88.559	-14.888
1400	5.358	55.283	50.662	6.469	133.976	85.059	-13.278
1500	5.333	55.652	50.983	7.003	133.745	81.572	-11.885
1600	5.318	55.996	51.287	7.535	133.500	78.100	-10.668
1700	5.311	56.318	51.573	8.067	133.241	74.647	-9.596
1800	5.310	56.621	51.844	8.598	132.969	71.207	-8.646
1900	5.316	56.909	52.104	9.129	132.684	67.782	-7.797
2000	5.326	57.182	52.351	9.661	132.389	64.375	-7.034
2042	5.331	57.293	52.452	9.885	132.260	62.947	-6.737
2042	5.331	57.293	52.452	9.885	127.564	62.947	-6.737
2100	5.339	57.442	52.588	10.194	127.392	61.114	-6.360
2200	5.356	57.691	52.814	10.729	127.096	57.965	-5.758

Phase change: 2042 K, melting point of Pt; ΔH° = 4.696 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2200 K: $C_p^\circ = 7.049 - 1.114\times10^{-3}T - 0.546\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.049\times10^{-3}T - 0.557\times10^{-6}T^2 + 0.546\times10^{5}T^{-2} - 2.235$

Formation equations (kcal/mol):

298.15-2042 K: $\Delta H_f^\circ = 134.664 + 1.223\times10^{-3}T - 1.187\times10^{-6}T^2 + 52.600T^{-1}$

$\Delta G_f^\circ = 134.664 - 1.223\times10^{-3}T\ln T + 1.187\times10^{-6}T^2 + 26.300T^{-1} - 28.231\times10^{-3}T$

2042-2200 K: $\Delta H_f^\circ = 132.392 - 1.251\times10^{-3}T - 0.557\times10^{-6}T^2 + 54.600T^{-1}$

$\Delta G_f^\circ = 132.392 + 1.251\times10^{-3}T\ln T + 0.557\times10^{-6}T^2 + 27.300T^{-1} - 44.688\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). All other data from Hilsenrath (94).

Pu(c,1)

Plutonium

T, K	cal/mol·K			$H^\circ - H^s_{298}$,
	Cp°	S°	$-(G^\circ - H^s_{298})/T$	kcal/mol
298.15	7.850	13.420	13.420	0
300	7.869	13.469	13.420	.015
395	9.253	15.796	13.718	.821
395	8.098	17.872	13.718	1.641
400	8.124	17.974	13.769	1.682
480	8.540	19.492	14.600	2.348
480	8.406	19.773	14.600	2.483
500	8.541	20.119	14.813	2.653
588	9.135	21.550	15.715	3.431
588	8.880	21.789	15.715	3.571
600	8.880	21.968	15.840	3.677
700	8.880	23.337	16.816	4.565
730	8.880	23.709	17.092	4.831
730	8.500	23.737	17.092	4.851
752	8.500	23.989	17.290	5.038
752	8.230	24.574	17.290	5.478
800	8.230	25.084	17.741	5.874
900	8.230	26.053	18.612	6.697
913	8.230	26.171	18.718	6.804
913	10.100	26.910	18.718	7.479
1000	10.100	27.830	19.473	8.357
1100	10.100	28.792	20.277	9.367
1200	10.100	29.671	21.024	10.377
1300*	10.100	30.479	21.720	11.387
1400	10.100	31.228	22.373	12.397
1500	10.100	31.925	22.987	13.407
1600	10.100	32.577	23.566	14.417
1700	10.100	33.189	24.114	15.427
1800	10.100	33.766	24.634	16.437
1900	10.100	34.312	25.129	17.447
2000	10.100	34.830	25.602	18.457
2100	10.100	35.323	26.053	19.467
2200	10.100	35.793	26.485	20.477
2300	10.100	36.242	26.900	21.487
2400	10.100	36.672	27.298	22.497
2500	10.100	37.084	27.681	23.507

*Data above 1200 K extrapolated.

Phase changes: 395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

Pu(c,l) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-395 K: $Cp^\circ = 3.990 + 12.948\times10^{-3}T$

$H^\circ - H^\circ_{298} = 3.990\times10^{-3}T + 6.474\times10^{-6}T^2 - 1.765$

395-480 K: $Cp^\circ = 6.057 + 5.168\times10^{-3}T$

$H^\circ - H^\circ_{298} = 6.057\times10^{-3}T + 2.584\times10^{-6}T^2 - 1.155$

480-588 K: $Cp^\circ = 5.102 + 6.884\times10^{-3}T$

$H^\circ - H^\circ_{298} = 5.102\times10^{-3}T + 3.442\times10^{-6}T^2 - 0.759$

588-730 K: $Cp^\circ = 8.877$

$H^\circ - H^\circ_{298} = 8.877\times10^{-3}T - 1.649$

730-752 K: $Cp^\circ = 8.500$

$H^\circ - H^\circ_{298} = 8.500\times10^{-3}T - 1.354$

752-913 K: $Cp^\circ = 8.232$

$H^\circ - H^\circ_{298} = 8.232\times10^{-3}T - 0.712$

913-2500 K: $Cp^\circ = 10.100$

$H^\circ - H^\circ_{298} = 10.100\times10^{-3}T - 1.742$

Source: Data from Oetting (167) who extrapolated above 1200 K by assuming constant heat capacity.

Pu(g)

Plutonium (ideal monatomic gas)

[Formation: Pu(c,1) = Pu(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH_f°	ΔG_f°	
298.15	4.984	42.317	42.317	0	82.500	73.884	-54.158
300	4.985	42.348	42.318	.009	82.494	73.830	-53.785
395	5.097	43.731	42.499	.486	82.166	71.131	-39.356
395	5.097	43.731	42.499	.486	81.346	71.131	-39.356
400	5.103	43.795	42.515	.512	81.330	71.002	-38.793
480	5.335	44.742	42.807	.929	81.081	68.961	-31.398
480	5.335	44.742	42.807	.929	80.946	68.961	-31.398
500	5.393	44.961	42.889	1.036	80.883	68.462	-29.924
588	5.771	45.864	43.268	1.526	80.595	66.299	-24.642
588	5.771	45.864	43.268	1.526	80.455	66.299	-24.642
600	5.823	45.981	43.321	1.596	80.419	66.011	-24.044
700	6.325	46.916	43.769	2.203	80.138	63.633	-19.867
730	6.480	47.185	43.904	2.395	80.064	62.927	-18.839
730	6.480	47.185	43.904	2.395	80.044	62.927	-18.839
752	6.594	47.378	44.003	2.539	80.001	62.412	-18.138
752	6.594	47.378	44.003	2.539	79.561	62.412	-18.138
800	6.842	47.794	44.218	2.861	79.487	61.319	-16.751
900	7.348	48.629	44.661	3.571	79.374	59.056	-14.340
913	7.412	48.735	44.718	3.667	79.363	58.762	-14.066
913	7.412	48.735	44.718	3.667	78.688	58.762	-14.066
1000	7.840	49.429	45.099	4.330	78.473	56.874	-12.430
1100	8.319	50.199	45.528	5.138	78.271	54.723	-10.872
1200	8.789	50.943	45.948	5.994	78.117	52.591	-9.578
1300	9.249	51.665	46.360	6.896	78.009	50.467	-8.484
1400	9.695	52.367	46.765	7.843	77.946	48.351	-7.548
1500	10.121	53.050	47.161	8.834	77.927	46.240	-6.737
1600	10.520	53.716	47.550	9.866	77.949	44.127	-6.027
1700	10.886	54.365	47.931	10.937	78.010	42.011	-5.401
1800	11.217	54.997	48.307	12.042	78.105	39.889	-4.843
1900	11.510	55.611	48.675	13.179	78.232	37.764	-4.344
2000	11.769	56.208	49.036	14.343	78.386	35.630	-3.893
2100	11.996	56.788	49.392	15.532	78.565	33.489	-3.485
2200	12.196	57.351	49.741	16.741	78.764	31.336	-3.113
2300	12.375	57.897	50.084	17.970	78.983	29.177	-2.772
2400	12.539	58.427	50.420	19.216	79.219	27.007	-2.459
2500	12.692	58.942	50.751	20.478	79.471	24.826	-2.170

Phase changes: 395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

Pu(g) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 3.075 + 4.588\times10^{-3}T + 0.481\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 3.075\times10^{-3}T + 2.294\times10^{-6}T^2 - 0.481\times10^{2}T^{-1} - 0.959$

2000-2500 K: $C_p^\circ = 12.844 + 0.440\times10^{-3}T - 78.200\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 12.844\times10^{-3}T + 0.220\times10^{-6}T^2 + 78.200\times10^{2}T^{-1} - 16.135$

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf^\circ = 83.306 - 0.915\times10^{-3}T - 4.180\times10^{-6}T^2 - 48.100T^{-1}$

$\Delta Gf^\circ = 83.306 + 0.915\times10^{-3}T\ln T + 4.180\times10^{-6}T^2 - 24.050T^{-1} - 37.788\times10^{-3}T$

395-480 K: $\Delta Hf^\circ = 82.695 - 2.982\times10^{-3}T - 0.290\times10^{-6}T^2 - 48.100T^{-1}$

$\Delta Gf^\circ = 82.695 + 2.982\times10^{-3}T\ln T + 0.290\times10^{-6}T^2 - 24.050T^{-1} - 47.065\times10^{-3}T$

480-588 K: $\Delta Hf^\circ = 82.300 - 2.027\times10^{-3}T - 1.148\times10^{-6}T^2 - 48.100T^{-1}$

$\Delta Gf^\circ = 82.300 + 2.027\times10^{-3}T\ln T + 1.148\times10^{-6}T^2 - 24.050T^{-1} - 40.756\times10^{-3}T$

588-730 K: $\Delta Hf^\circ = 83.189 - 5.802\times10^{-3}T + 2.294\times10^{-6}T^2 - 48.100T^{-1}$

$\Delta Gf^\circ = 83.189 + 5.802\times10^{-3}T\ln T - 2.294\times10^{-6}T^2 - 24.050T^{-1} - 64.317\times10^{-3}T$

730-752 K: $\Delta Hf^\circ = 82.894 - 5.425\times10^{-3}T + 2.294\times10^{-6}T^2 - 48.100T^{-1}$

$\Delta Gf^\circ = 82.894 + 5.425\times10^{-3}T\ln T - 2.294\times10^{-6}T^2 - 24.050T^{-1} - 61.427\times10^{-3}T$

752-913 K: $\Delta Hf^\circ = 82.252 - 5.157\times10^{-3}T + 2.294\times10^{-6}T^2 - 48.100T^{-1}$

$\Delta Gf^\circ = 82.252 + 5.157\times10^{-3}T\ln T - 2.294\times10^{-6}T^2 - 24.050T^{-1} - 58.799\times10^{-3}T$

913-2000 K: $\Delta Hf^\circ = 83.283 - 7.025\times10^{-3}T + 2.294\times10^{-6}T^2 - 48.100T^{-1}$

$\Delta Gf^\circ = 83.283 + 7.025\times10^{-3}T\ln T - 2.294\times10^{-6}T^2 - 24.050T^{-1} - 72.662\times10^{-3}T$

2000-2500 K: $\Delta Hf^\circ = 68.107 + 2.744\times10^{-3}T + 0.220\times10^{-6}T^2 + 7820.000T^{-1}$

$\Delta Gf^\circ = 68.107 - 2.744\times10^{-3}T\ln T - 0.220\times10^{-6}T^2 + 3910.000T^{-1} + 4.048\times10^{-3}T$

Source: Data from Oetting (167).

PuO(c)

Plutonium Oxide

[Formation: $Pu(c,l) + 0.5O_2(g) = PuO(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	12.250	16.900	16.900	0	-135.000	-128.732	94.362
300	12.270	16.976	16.900	.023	-134.999	-128.693	93.752
395	12.859	20.431	17.348	1.218	-134.947	-126.705	70.104
395	12.859	20.431	17.348	1.218	-135.767	-126.705	70.104
400	12.890	20.593	17.388	1.282	-135.762	-126.591	69.165
480	13.306	22.982	18.128	2.330	-135.671	-124.766	56.807
480	13.306	22.982	18.128	2.330	-135.806	-124.766	56.807
500	13.410	23.527	18.333	2.597	-135.783	-124.307	54.334
588	13.788	25.731	19.278	3.794	-135.695	-122.294	45.454
588	13.788	25.731	19.278	3.794	-135.835	-122.294	45.454
600	13.840	26.010	19.410	3.960	-135.821	-122.018	44.444
700	14.250	28.175	20.511	5.365	-135.693	-119.726	37.380
730	14.355	28.775	20.838	5.794	-135.649	-119.043	35.639
730	14.355	28.775	20.838	5.794	-135.669	-119.043	35.639
752	14.432	29.203	21.076	6.111	-135.627	-118.543	34.451
752	14.432	29.203	21.076	6.111	-136.067	-118.543	34.451
800	14.600	30.101	21.591	6.808	-135.958	-117.428	32.079
900	14.930	31.840	22.634	8.285	-135.712	-115.126	27.956
913	14.966	32.054	22.767	8.479	-135.678	-114.829	27.487
913	14.966	32.054	22.767	8.479	-136.353	-114.829	27.487
1000	15.210	33.428	23.636	9.792	-136.278	-112.781	24.648
1100	15.480	34.890	24.594	11.326	-136.174	-110.437	21.941
1200	15.720	36.248	25.509	12.887	-136.046	-108.102	19.688
1300	15.940	37.515	26.384	14.470	-135.902	-105.780	17.783
1400	16.140	38.704	27.223	16.074	-135.740	-103.469	16.152
1500	16.300	39.823	28.026	17.696	-135.563	-101.170	14.740
1600	16.460	40.880	28.796	19.334	-135.373	-98.883	13.507
1700	16.600	41.882	29.537	20.987	-135.171	-96.608	12.420
1800	16.720	42.834	30.249	22.653	-134.959	-94.346	11.455
1900	16.830	43.741	30.935	24.331	-134.738	-92.095	10.593
2000	16.950	44.608	31.598	26.020	-134.508	-89.858	9.819
2100	17.010	45.436	32.237	27.718	-134.273	-87.630	9.120
2173	17.050	46.018	32.690	28.961	-134.099	-86.012	8.651

*All data estimated.

Phase changes: 395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.
2173 K, melting point of PuO.

PuO(c) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2173 K: $C_p^\circ = 12.692 + 2.440\times10^{-3}T - 1.039\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 12.692\times10^{-3}T + 1.220\times10^{-6}T^2 + 1.039\times10^{2}T^{-1} - 4.241$

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf^\circ = -136.300 + 5.087\times10^{-3}T - 5.505\times10^{-6}T^2 + 81.300T^{-1}$

$\Delta Gf^\circ = -136.300 - 5.087\times10^{-3}T\ln T + 5.505\times10^{-6}T^2 + 40.650T^{-1} + 52.268\times10^{-3}T$

395-480 K: $\Delta Hf^\circ = -136.910 + 3.020\times10^{-3}T - 1.616\times10^{-6}T^2 + 81.300T^{-1}$

$\Delta Gf^\circ = -136.910 - 3.020\times10^{-3}T\ln T + 1.616\times10^{-6}T^2 + 40.650T^{-1} + 42.991\times10^{-3}T$

480-588 K: $\Delta Hf^\circ = -137.306 + 3.975\times10^{-3}T - 2.474\times10^{-6}T^2 + 81.300T^{-1}$

$\Delta Gf^\circ = -137.306 - 3.975\times10^{-3}T\ln T + 2.474\times10^{-6}T^2 + 40.650T^{-1} + 49.300\times10^{-3}T$

588-730 K: $\Delta Hf^\circ = -136.417 + 0.200\times10^{-3}T + 0.969\times10^{-6}T^2 + 81.300T^{-1}$

$\Delta Gf^\circ = -136.417 - 0.200\times10^{-3}T\ln T - 0.969\times10^{-6}T^2 + 40.650T^{-1} + 25.738\times10^{-3}T$

730-752 K: $\Delta Hf^\circ = -136.712 + 0.577\times10^{-3}T + 0.969\times10^{-6}T^2 + 81.300T^{-1}$

$\Delta Gf^\circ = -136.712 - 0.577\times10^{-3}T\ln T - 0.969\times10^{-6}T^2 + 40.650T^{-1} + 28.628\times10^{-3}T$

752-913 K: $\Delta Hf^\circ = -137.353 + 0.845\times10^{-3}T + 0.969\times10^{-6}T^2 + 81.300T^{-1}$

$\Delta Gf^\circ = -137.353 - 0.845\times10^{-3}T\ln T - 0.969\times10^{-6}T^2 + 40.650T^{-1} + 31.256\times10^{-3}T$

913-2000 K: $\Delta Hf^\circ = -136.323 - 1.023\times10^{-3}T + 0.969\times10^{-6}T^2 + 81.300T^{-1}$

$\Delta Gf^\circ = -136.323 + 1.023\times10^{-3}T\ln T - 0.969\times10^{-6}T^2 + 40.650T^{-1} + 17.394\times10^{-3}T$

2000-2173 K: $\Delta Hf^\circ = -135.655 - 1.578\times10^{-3}T + 1.115\times10^{-6}T^2 - 211.100T^{-1}$

$\Delta Gf^\circ = -135.655 + 1.578\times10^{-3}T\ln T - 1.115\times10^{-6}T^2 - 105.550T^{-1} + 13.172\times10^{-3}T$

Source: Data are those estimated by Oetting (166).

$PuO_2(c)$

Plutonium Dioxide

[Formation: $Pu(c,l) + O_2(g) = PuO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	15.834	15.805	15.805	0	-252.350	-238.450	174.786
300	15.911	15.903	15.806	.029	-252.349	-238.364	173.646
395	18.564	20.703	16.419	1.692	-252.166	-233.960	129.446
395	18.564	20.703	16.419	1.692	-252.986	-233.960	129.446
400	18.704	20.937	16.475	1.785	-252.970	-233.719	127.697
480	19.673	24.448	17.516	3.327	-252.677	-229.895	104.673
480	19.673	24.448	17.516	3.327	-252.812	-229.895	104.673
500	19.915	25.256	17.810	3.723	-252.734	-228.942	100.069
588	20.491	28.535	19.175	5.504	-252.394	-224.783	83.547
588	20.491	28.535	19.175	5.504	-252.534	-224.783	83.547
600	20.569	28.950	19.367	5.750	-252.486	-224.217	81.670
700	20.979	32.153	20.969	7.829	-252.073	-219.537	68.542
730	21.069	33.035	21.447	8.460	-251.946	-218.145	65.308
730	21.069	33.035	21.447	8.460	-251.966	-218.145	65.308
752	21.135	33.663	21.794	8.925	-251.863	-217.128	63.102
752	21.135	33.663	21.794	8.925	-252.303	-217.128	63.102
800	21.279	34.975	22.546	9.943	-252.066	-214.891	58.705
900	21.531	37.496	24.070	12.083	-251.563	-210.275	51.061
913	21.562	37.805	24.264	12.363	-251.497	-209.679	50.191
913	21.562	37.805	24.264	12.363	-252.172	-209.679	50.191
1000	21.767	39.777	25.529	14.248	-251.885	-205.642	44.942
1100	22.007	41.863	26.920	16.437	-251.545	-201.034	39.941
1200	22.261	43.788	28.246	18.650	-251.190	-196.457	35.779
1300	22.536	45.581	29.512	20.890	-250.816	-191.912	32.263
1400	22.838	47.262	30.721	23.158	-250.422	-187.395	29.253
1500	23.169	48.849	31.877	25.458	-250.002	-182.909	26.649
1600	23.531	50.355	32.984	27.793	-249.554	-178.448	24.375
1700	23.926	51.794	34.049	30.166	-249.073	-174.020	22.371
1800	24.354	53.173	35.074	32.579	-248.558	-169.619	20.594
1900	24.817	54.502	36.061	35.038	-248.003	-165.249	19.008
2000	25.315	55.788	37.016	37.544	-247.406	-160.910	17.583
2100	25.849	57.036	37.940	40.102	-246.763	-156.599	16.297
2200	26.418	58.251	38.835	42.715	-246.070	-152.321	15.132
2300	27.022	59.439	39.706	45.387	-245.324	-148.078	14.070
2400	27.663	60.602	40.552	48.121	-244.521	-143.865	13.101
2500	28.339	61.745	41.377	50.920	-243.658	-139.691	12.212

Phase changes: 395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.
2715 K, melting point of PuO_2; ΔH° = 18. kcal/mol.

PuO_2(c) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 20.677 + 1.906\times10^{-3}T - 4.810\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 20.677\times10^{-3}T + 0.953\times10^{-6}T^2 + 4.810\times10^{2}T^{-1} - 7.863$

2000-2500 K: $C_p^\circ = 13.204 + 6.048\times10^{-3}T$

$H^\circ - H^\circ_{298} = 13.204\times10^{-3}T + 3.024\times10^{-6}T^2 - 0.960$

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf^\circ = -256.096 + 9.457\times10^{-3}T - 6.024\times10^{-6}T^2 + 435.800T^{-1}$

$\Delta Gf^\circ = -256.096 - 9.457\times10^{-3}T\ln T + 6.024\times10^{-6}T^2 + 217.900T^{-1} + 108.818\times10^{-3}T$

395-480 K: $\Delta Hf^\circ = -256.706 + 7.390\times10^{-3}T - 2.134\times10^{-6}T^2 + 435.800T^{-1}$

$\Delta Gf^\circ = -256.706 - 7.390\times10^{-3}T\ln T + 2.134\times10^{-6}T^2 + 217.900T^{-1} + 99.542\times10^{-3}T$

480-588 K: $\Delta Hf^\circ = -257.102 + 8.345\times10^{-3}T - 2.992\times10^{-6}T^2 + 435.800T^{-1}$

$\Delta Gf^\circ = -257.102 - 8.345\times10^{-3}T\ln T + 2.992\times10^{-6}T^2 + 217.900T^{-1} + 105.850\times10^{-3}T$

588-730 K: $\Delta Hf^\circ = -256.212 + 4.570\times10^{-3}T + 0.450\times10^{-6}T^2 + 435.800T^{-1}$

$\Delta Gf^\circ = -256.212 - 4.570\times10^{-3}T\ln T - 0.450\times10^{-6}T^2 + 217.900T^{-1} + 82.289\times10^{-3}T$

730-752 K: $\Delta Hf^\circ = -256.508 + 4.947\times10^{-3}T + 0.450\times10^{-6}T^2 + 435.800T^{-1}$

$\Delta Gf^\circ = -256.508 - 4.947\times10^{-3}T\ln T - 0.450\times10^{-6}T^2 + 217.900T^{-1} + 85.179\times10^{-3}T$

752-913 K: $\Delta Hf^\circ = -257.149 + 5.215\times10^{-3}T + 0.450\times10^{-6}T^2 + 435.800T^{-1}$

$\Delta Gf^\circ = -257.149 - 5.215\times10^{-3}T\ln T - 0.450\times10^{-6}T^2 + 217.900T^{-1} + 87.807\times10^{-3}T$

913-2000 K: $\Delta Hf^\circ = -256.119 + 3.347\times10^{-3}T + 0.450\times10^{-6}T^2 + 435.800T^{-1}$

$\Delta Gf^\circ = -256.119 - 3.347\times10^{-3}T\ln T - 0.450\times10^{-6}T^2 + 217.900T^{-1} + 73.945\times10^{-3}T$

2000-2500 K: $\Delta Hf^\circ = -247.880 - 5.236\times10^{-3}T + 2.815\times10^{-6}T^2 - 630.000T^{-1}$

$\Delta Gf^\circ = -247.880 + 5.236\times10^{-3}T\ln T - 2.815\times10^{-6}T^2 - 315.000T^{-1} + 9.450\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (106). Low-temperature heat capacities and entropy at 298 K from Flotow (67). High-temperature data based on Kruger (140) and Ogard (168). Temperature and enthalpy of fusion estimated by Ogard (168) using incomplete data.

$Pu_2O_3(\alpha)$

Diplutonium Trioxide, Plutonium Sesquioxide

[Formation: $2Pu(c,l) + 1.5O_2(g) = Pu_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	31.800	36.700	36.700	0	-430.000	-411.023	301.284
300	32.000	36.897	36.700	.059	-429.991	-410.906	299.341
395	35.325	46.174	37.895	3.270	-429.403	-404.945	224.049
395	35.325	46.174	37.895	3.270	-431.043	-404.945	224.049
400	35.500	46.619	38.001	3.447	-431.001	-404.616	221.069
480	37.068	53.242	40.003	6.355	-430.300	-399.402	181.850
480	37.068	53.242	40.003	6.355	-430.570	-399.402	181.850
500	37.460	54.763	40.563	7.100	-430.387	-398.109	174.011
588	38.657	60.934	43.160	10.451	-429.587	-392.495	145.882
588	38.657	60.934	43.160	10.451	-429.867	-392.495	145.882
600	38.820	61.717	43.524	10.916	-429.752	-391.733	142.687
700	39.900	67.785	46.565	14.854	-428.757	-385.473	120.349
730	40.158	69.465	47.472	16.055	-428.444	-383.624	114.849
730	40.158	69.465	47.472	16.055	-428.484	-383.624	114.849
752	40.347	70.661	48.132	16.941	-428.235	-382.278	111.098
752	40.347	70.661	48.132	16.941	-429.115	-382.278	111.098
800	40.760	73.170	49.560	18.888	-428.538	-379.307	103.621
900	41.560	78.017	52.457	23.004	-427.289	-373.228	90.631
913	41.656	78.614	52.825	23.545	-427.122	-372.449	89.154
913	41.656	78.614	52.825	23.545	-428.472	-372.449	89.154
1000	42.300	82.435	55.238	27.197	-427.656	-367.146	80.239
1100	43.000	86.500	57.896	31.464	-426.668	-361.142	71.751
1200	43.560	90.266	60.439	35.792	-425.632	-355.230	64.695
1300	44.100	93.775	62.870	40.176	-424.552	-349.408	58.740
1400	44.520	97.058	65.196	44.607	-423.437	-343.668	53.648
1500	44.940	100.144	67.424	49.080	-422.289	-338.010	49.247
1600	45.300	103.056	69.561	53.592	-421.112	-332.430	45.407
1700	45.640	105.813	71.613	58.140	-419.907	-326.924	42.028
1800	45.940	108.430	73.586	62.719	-418.680	-321.489	39.034
1900	46.220	110.922	75.487	67.327	-417.433	-316.126	36.362
2000	46.460	113.299	77.319	71.961	-416.168	-310.827	33.965

*All data except enthalpy of formation and entropy at 298 K estimated.

Phase changes: 395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

$Pu_2O_3(\alpha)$ - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 37.424 + 5.320\times10^{-3}T - 6.409\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 37.424\times10^{-3}T + 2.660\times10^{-6}T^2 + 6.409\times10^{2}T^{-1} - 13.544$

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf^\circ = -436.486 + 18.599\times10^{-3}T - 11.042\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -436.486 - 18.599\times10^{-3}T\ln T + 11.042\times10^{-6}T^2 + 286.550T^{-1} + 184.855\times10^{-3}T$

395-480 K: $\Delta Hf^\circ = -437.707 + 14.465\times10^{-3}T - 3.262\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -437.707 - 14.465\times10^{-3}T\ln T + 3.262\times10^{-6}T^2 + 286.550T^{-1} + 166.302\times10^{-3}T$

480-588 K: $\Delta Hf^\circ = -438.498 + 16.375\times10^{-3}T - 4.979\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -438.498 - 16.375\times10^{-3}T\ln T + 4.979\times10^{-6}T^2 + 286.550T^{-1} + 178.919\times10^{-3}T$

588-730 K: $\Delta Hf^\circ = -436.719 + 8.825\times10^{-3}T + 1.906\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -436.719 - 8.825\times10^{-3}T\ln T - 1.906\times10^{-6}T^2 + 286.550T^{-1} + 131.797\times10^{-3}T$

730-752 K: $\Delta Hf^\circ = -437.309 + 9.579\times10^{-3}T + 1.906\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -437.309 - 9.579\times10^{-3}T\ln T - 1.906\times10^{-6}T^2 + 286.550T^{-1} + 137.577\times10^{-3}T$

752-913 K: $\Delta Hf^\circ = -438.592 + 10.115\times10^{-3}T + 1.906\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -438.592 - 10.115\times10^{-3}T\ln T - 1.906\times10^{-6}T^2 + 286.550T^{-1} + 142.833\times10^{-3}T$

913-2000 K: $\Delta Hf^\circ = -436.531 + 6.379\times10^{-3}T + 1.906\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -436.531 - 6.379\times10^{-3}T\ln T - 1.906\times10^{-6}T^2 + 286.550T^{-1} + 115.108\times10^{-3}T$

Source: Data from Oetting (166) who estimated all except enthalpy of formation and entropy at 298 K.

$Pu_2O_3(\beta)$

Diplutonium Trioxide, Plutonium Sesquioxide

[Formation: $2Pu(c,l) + 1.5O_2(g) = Pu_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	31.300	33.200	33.200	0	-410.000	-389.980	285.859
300	31.500	33.394	33.201	.058	-409.991	-389.856	284.006
395	34.825	42.533	34.377	3.221	-409.451	-383.556	212.215
395	34.825	42.533	34.377	3.221	-411.091	-383.556	212.215
400	35.000	42.972	34.482	3.396	-411.052	-383.208	209.372
480	36.568	49.503	36.454	6.264	-410.391	-377.699	171.969
480	36.568	49.503	36.454	6.264	-410.661	-377.699	171.969
500	36.960	51.004	37.006	6.999	-410.488	-376.330	164.492
588	38.157	57.094	39.567	10.306	-409.732	-370.382	137.663
588	38.157	57.094	39.567	10.306	-410.012	-370.382	137.663
600	38.320	57.867	39.925	10.765	-409.902	-369.574	134.615
700	39.400	63.858	42.925	14.653	-408.958	-362.926	113.309
730	39.658	65.517	43.820	15.839	-408.660	-360.958	108.063
730	39.658	65.517	43.820	15.839	-408.700	-360.958	108.063
752	39.847	66.698	44.471	16.714	-408.462	-359.525	104.485
752	39.847	66.698	44.471	16.714	-409.342	-359.525	104.485
800	40.260	69.176	45.880	18.637	-408.789	-356.363	97.353
900	41.060	73.965	48.739	22.703	-407.590	-349.882	84.962
913	41.156	74.555	49.103	23.237	-407.429	-349.050	83.553
913	41.156	74.555	49.103	23.237	-408.779	-349.050	83.553
1000	41.800	78.330	51.484	26.846	-408.007	-343.392	75.047
1100	42.500	82.347	54.108	31.063	-407.069	-336.974	66.950
1200	43.060	86.070	56.619	35.341	-406.082	-330.646	60.218
1300	43.600	89.538	59.019	39.675	-405.053	-324.401	54.536
1400	44.020	92.785	61.316	44.056	-403.988	-318.237	49.678
1500	44.440	95.837	63.518	48.479	-402.889	-312.151	45.480
1600	44.800	98.716	65.628	52.941	-401.763	-306.137	41.816
1700	45.140	101.448	67.660	57.439	-400.608	-300.204	38.593
1800	45.440	104.031	69.604	61.968	-399.431	-294.322	35.735
1900	45.720	106.496	71.482	66.526	-398.234	-288.518	33.187
2000	45.960	108.847	73.292	71.110	-397.019	-282.775	30.900

*All data except enthalpy of formation and entropy at 298 K estimated.

Phase changes: 395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

$Pu_2O_3(\beta)$ - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 36.924 + 5.320\times10^{-3}T - 6.409\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 36.924\times10^{-3}T + 2.660\times10^{-6}T^2 + 6.409\times10^{2}T^{-1} - 13.395$

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf^\circ = -416.337 + 18.099\times10^{-3}T - 11.042\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -416.337 - 18.099\times10^{-3}T\ln T + 11.042\times10^{-6}T^2 + 286.550T^{-1} + 185.006\times10^{-3}T$

395-480 K: $\Delta Hf^\circ = -417.558 + 13.965\times10^{-3}T - 3.262\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -417.558 - 13.965\times10^{-3}T\ln T + 3.262\times10^{-6}T^2 + 286.550T^{-1} + 166.453\times10^{-3}T$

480-588 K: $\Delta Hf^\circ = -418.349 + 15.875\times10^{-3}T - 4.979\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -418.349 - 15.875\times10^{-3}T\ln T + 4.979\times10^{-6}T^2 + 286.550T^{-1} + 179.071\times10^{-3}T$

588-730 K: $\Delta Hf^\circ = -416.570 + 8.325\times10^{-3}T + 1.906\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -416.570 - 8.325\times10^{-3}T\ln T - 1.906\times10^{-6}T^2 + 286.550T^{-1} + 131.948\times10^{-3}T$

730-752 K: $\Delta Hf^\circ = -417.160 + 9.079\times10^{-3}T + 1.906\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -417.160 - 9.079\times10^{-3}T\ln T - 1.906\times10^{-6}T^2 + 286.550T^{-1} + 137.728\times10^{-3}T$

752-913 K: $\Delta Hf^\circ = -418.443 + 9.615\times10^{-3}T + 1.906\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -418.443 - 9.615\times10^{-3}T\ln T - 1.906\times10^{-6}T^2 + 286.550T^{-1} + 142.984\times10^{-3}T$

913-2000 K: $\Delta Hf^\circ = -416.382 + 5.879\times10^{-3}T + 1.906\times10^{-6}T^2 + 573.100T^{-1}$

$\Delta Gf^\circ = -416.382 - 5.879\times10^{-3}T\ln T - 1.906\times10^{-6}T^2 + 286.550T^{-1} + 115.259\times10^{-3}T$

Source: Data from Oetting (166) who estimated all except enthalpy of formation and entropy at 298 K.

Rb(c,l,g)

Rubidium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	7.424	18.350	18.350	0
300	7.465	18.396	18.350	.014
312.64	7.744	18.710	18.358	.110
312.64	8.222	20.386	18.358	.634
400	7.856	22.371	19.031	1.336
500	7.510	24.081	19.873	2.104
600	7.251	25.426	20.691	2.841
700	7.057	26.529	21.449	3.556
800	6.932	27.463	22.144	4.255
900	6.881	28.283	22.789	4.945
974.5	6.900	28.829	23.226	5.460
974.5	4.968	46.510	23.226	22.690
1000	4.968	46.638	23.821	22.817
1100	4.968	47.112	25.917	23.314
1200	4.968	47.544	27.701	23.811
1300	4.969	47.942	29.244	24.307
1400	4.970	48.310	30.593	24.804
1500	4.972	48.653	31.786	25.301
1600	4.976	48.974	32.850	25.799
1700	4.983	49.276	33.807	26.297
1800	4.992	49.561	34.675	26.795
1900	5.005	49.831	35.465	27.295
2000	5.022	50.088	36.190	27.797

Phase changes: 312.64 K, melting point of Rb; ΔH° = 0.524 kcal/mol.
974.5 K, calculated boiling point to ideal monatomic gas; ΔH° = 17.230 kcal/mol.
961 K, normal boiling point to equilibrium mixture of Rb(g) and Rb_2(g).

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-312.64 K: $Cp^\circ = 0.533 + 23.112\times10^{-3}T$

$H^\circ - H^\circ_{298} = 0.533\times10^{-3}T + 11.556\times10^{-6}T^2 - 1.186$

312.64-974.5 K: $Cp^\circ = 7.873 - 1.276\times10^{-3}T + 0.732\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.873\times10^{-3}T - 0.638\times10^{-6}T^2 - 0.732\times10^{2}T^{-1} - 1.531$

974.5-2000 K: $Cp^\circ = 4.990 - 0.004\times10^{-3}T - 0.179\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.990\times10^{-3}T - 0.002\times10^{-6}T^2 + 0.179\times10^{2}T^{-1} + 17.811$

Source: Data from Hultgren (99).

Rb(g)

Rubidium (ideal monatomic gas)

[Formation: Rb(c,l,g) = Rb(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	40.626	40.626	0	19.330	12.688	-9.301
300	4.968	40.657	40.627	.009	19.325	12.647	-9.213
312.64	4.968	40.862	40.632	.072	19.292	12.366	-8.644
312.64	4.968	40.862	40.632	.072	18.768	12.366	-8.644
400	4.968	42.086	40.821	.506	18.500	10.614	-5.799
500	4.968	43.194	41.188	1.003	18.229	8.672	-3.791
600	4.968	44.100	41.600	1.500	17.989	6.785	-2.471
700	4.968	44.866	42.015	1.996	17.770	4.934	-1.540
800	4.968	45.529	42.413	2.493	17.568	3.115	-.851
900	4.968	46.114	42.792	2.990	17.375	1.327	-.322
974.5	4.968	46.510	43.061	3.360	17.230	0	0
974.5	4.968	46.510	43.061	3.360	0	0	0
1000	4.968	46.638	43.151	3.487	0	0	0
1100	4.968	47.112	43.490	3.984	0	0	0
1200	4.968	47.544	43.810	4.481	0	0	0
1300	4.969	47.942	44.114	4.977	0	0	0
1400	4.970	48.310	44.400	5.474	0	0	0
1500	4.972	48.653	44.672	5.971	0	0	0
1600	4.976	48.974	44.931	6.469	0	0	0
1700	4.983	49.276	45.178	6.967	0	0	0
1800	4.992	49.561	45.414	7.465	0	0	0
1900	5.005	49.831	45.639	7.965	0	0	0
2000	5.022	50.088	45.854	8.467	0	0	0

Phase changes: 312.64 K, melting point of Rb; $\Delta H° = 0.524$ kcal/mol.
974.5 K, boiling point of Rb to ideal monatomic gas; $\Delta H° = 17.230$ kcal/mol of Rb.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.963 + 0.006\times10^{-3}T + 0.003\times10^{5}T^{-2}$

$H°- H°_{298} = 4.963\times10^{-3}T + 0.003\times10^{-6}T^{2} - 0.003\times10^{2}T^{-1} - 1.479$

Formation equations (kcal/mol):

298.15-312.64 K: $\Delta Hf° = 19.037 + 4.430\times10^{-3}T - 11.553\times10^{-6}T^{2} - 0.300T^{-1}$

$\Delta Gf° = 19.037 - 4.430\times10^{-3}T\ln T + 11.553\times10^{-6}T^{2} - 0.150T^{-1} + 0.504\times10^{-3}T$

312.64-974.5 K: $\Delta Hf° = 19.382 - 2.910\times10^{-3}T + 0.641\times10^{-6}T^{2} + 72.900T^{-1}$

$\Delta Gf° = 19.382 + 2.910\times10^{-3}T\ln T - 0.641\times10^{-6}T^{2} + 36.450T^{-1} - 39.330\times10^{-3}T$

974.5-2000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Source: Data from Hultgren (99).

$RbO_2(c)$

Rubidium Dioxide, Rubidium Superoxide

[Formation: $Rb(c,l) + O_2(g) = RbO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.540	31.090	31.090	0	-66.600	-55.788	40.893
300*	18.570	31.205	31.092	.034	-66.593	-55.721	40.592
312.64	18.733	31.975	31.112	.270	-66.542	-55.264	38.631
312.64	18.733	31.975	31.112	.270	-67.066	-55.264	38.631
400	19.861	36.738	31.835	1.961	-66.698	-52.009	28.416
500	20.721	41.268	33.282	3.993	-66.165	-48.398	21.154
600	21.346	45.104	34.942	6.097	-65.553	-44.902	16.355

*Data above 298 K estimated.

Phase change: 312.64 K, melting point of Rb; $\Delta H° = 0.524$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 18.883 + 4.938\times10^{-3}T - 1.614\times10^{5}T^{-2}$

$H°- H°_{298} = 18.883\times10^{-3}T + 2.469\times10^{-6}T^{2} + 1.614\times10^{2}T^{-1} - 6.391$

Formation equations (kcal/mol):

298.15-312.64 K: $\Delta Hf° = -69.453 + 11.120\times10^{-3}T - 9.590\times10^{-6}T^{2} + 116.200T^{-1}$

$\Delta Gf° = -69.453 - 11.120\times10^{-3}T\ln T + 9.590\times10^{-6}T^{2} + 58.100T^{-1} + 105.677\times10^{-3}T$

312.64-600 K: $\Delta Hf° = -69.108 + 3.780\times10^{-3}T + 2.604\times10^{-6}T^{2} + 189.400T^{-1}$

$\Delta Gf° = -69.108 - 3.780\times10^{-3}T\ln T - 2.604\times10^{-6}T^{2} + 94.700T^{-1} + 65.844\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (239). Low-temperature heat capacities and entropy at 298 K from Paukov (184). High-temperature data estimated.

Re(c)

Rhenium

T, K	cal/mol•K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.035	8.730	8.730	0
300	6.039	8.767	8.730	.011
400	6.188	10.527	8.970	.623
500	6.314	11.921	9.425	1.248
600	6.441	13.083	9.940	1.886
700	6.571	14.086	10.463	2.536
800	6.703	14.972	10.972	3.200
900	6.834	15.769	11.461	3.877
1000	6.965	16.496	11.929	4.567
1100	7.095	17.166	12.375	5.270
1200	7.225	17.789	12.801	5.986
1300	7.355	18.372	13.207	6.715
1400	7.485	18.922	13.596	7.457
1500	7.615	19.443	13.968	8.212
1600	7.745	19.938	14.325	8.980
1700	7.875	20.412	14.670	9.761
1800	8.005	20.866	15.002	10.555
1900	8.135	21.302	15.322	11.362
2000	8.265	21.723	15.632	12.182

Phase change: 3453 K, melting point of Re; ΔH° = 7.9 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 5.676 + 1.292\times10^{-3}T - 0.024\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.676\times10^{-3}T + 0.646\times10^{-6}T^{2} + 0.024\times10^{2}T^{-1} - 1.758$

Source: Data from Hultgren (99).

Re(g)

Rhenium (ideal monatomic gas)

[Formation: Re(c) = Re(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	45.131	45.131	0	184.000	173.147	-126.919
300	4.968	45.162	45.132	.009	183.998	173.080	-126.087
400	4.968	46.591	45.326	.506	183.883	169.457	-92.586
500	4.968	47.700	45.694	1.003	183.755	165.866	-72.499
600	4.968	48.606	46.106	1.500	183.614	162.300	-59.117
700	4.968	49.371	46.520	1.996	183.460	158.761	-49.567
800	4.968	50.035	46.919	2.493	183.293	155.243	-42.410
900	4.968	50.620	47.298	2.990	183.113	151.747	-36.849
1000	4.968	51.143	47.656	3.487	182.920	148.273	-32.405
1100	4.968	51.617	47.995	3.984	182.714	144.818	-28.772
1200	4.969	52.049	48.316	4.480	182.494	141.382	-25.749
1300	4.970	52.447	48.619	4.977	182.262	137.965	-23.194
1400	4.974	52.815	48.904	5.475	182.018	134.568	-21.007
1500	4.979	53.159	49.178	5.972	181.760	131.186	-19.114
1600	4.989	53.480	49.436	6.470	181.490	127.823	-17.460
1700	5.003	53.783	49.683	6.970	181.209	124.478	-16.003
1800	5.025	54.070	49.919	7.471	180.916	121.149	-14.709
1900	5.056	54.342	50.145	7.975	180.613	117.837	-13.554
2000	5.097	54.602	50.361	8.483	180.301	114.543	-12.517

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.934 + 0.038\times10^{-3}T + 0.021\times10^{5}T^{-2}$

$H°- H°_{298} = 4.934\times10^{-3}T + 0.019\times10^{-6}T^{2} - 0.021\times10^{2}T^{-1} - 1.466$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 184.292 - 0.742\times10^{-3}T - 0.627\times10^{-6}T^{2} - 4.500T^{-1}$

$\Delta Gf° = 184.292 + 0.742\times10^{-3}T\ln T + 0.627\times10^{-6}T^{2} - 2.250T^{-1} - 41.770\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). All other data from Hilsenrath (94).

$ReO_2(c)$

Rhenium Dioxide

[Formation: $Re(c) + O_2(g) = ReO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.994	11.431	11.431	0	-107.300	-93.494	68.532
300	13.039	11.511	11.431	.024	-107.300	-93.409	68.047
400	14.905	15.539	11.966	1.429	-107.217	-88.786	48.510
500	16.191	19.012	13.038	2.987	-107.015	-84.200	36.803
600	17.082	22.048	14.291	4.654	-106.741	-79.662	29.016
700	17.696	24.730	15.596	6.394	-106.429	-75.173	23.470
800	18.137	27.123	16.889	8.187	-106.098	-70.731	19.323
900	18.486	29.280	18.148	10.019	-105.757	-66.330	16.107
1000	18.805	31.245	19.362	11.883	-105.410	-61.969	13.543
1100	19.137	33.052	20.525	13.780	-105.055	-57.641	11.452
1200	19.506	34.733	21.640	15.712	-104.687	-53.346	9.716
1300	19.916	36.310	22.708	17.683	-104.301	-49.084	8.252
1400	20.350	37.802	23.733	19.696	-103.894	-44.852	7.002

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp° = 16.002 + 3.200\times10^{-3}T - 3.522\times10^{5}T^{-2}$

$H°- H°_{298} = 16.002\times10^{-3}T + 1.600\times10^{-6}T^{2} + 3.522\times10^{2}T^{-1} - 6.095$

Formation equations (kcal/mol):

298.15-1400 K: $\Delta Hf° = -109.285 + 3.096\times10^{-3}T + 0.451\times10^{-6}T^{2} + 304.600T^{-1}$

$\Delta Gf° = -109.285 - 3.096\times10^{-3}T\ln T - 0.451\times10^{-6}T^{2} + 152.300T^{-1} + 69.022\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from King (133). All other data from Stuve (214).

$ReO_3(c)$

Rhenium Trioxide

[Formation: $Re(c) + 1.5O_2(g) = ReO_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.775	16.553	16.553	0	-140.800	-121.216	88.853
300	17.837	16.663	16.553	.033	-140.798	-121.094	88.216
400	20.380	22.177	17.287	1.956	-140.552	-114.558	62.591
500	21.995	26.909	18.751	4.079	-140.150	-108.103	47.251
600	23.175	31.028	20.461	6.340	-139.660	-101.739	37.058
700	24.088	34.672	22.236	8.705	-139.111	-95.461	29.804
800	24.806	37.937	23.998	11.151	-138.527	-89.267	24.386
900	25.361	40.892	25.713	13.661	-137.915	-83.145	20.190
1000	25.772	43.587	27.368	16.219	-137.287	-77.093	16.848

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 20.293 + 6.476\times10^{-3}T - 3.950\times10^{5}T^{-2}$

$H°- H°_{298} = 20.293\times10^{-3}T + 3.238\times10^{-6}T^{2} + 3.950\times10^{2}T^{-1} - 7.663$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf° = -143.177 + 3.772\times10^{-3}T + 1.837\times10^{-6}T^{2} + 324.800T^{-1}$

$\Delta Gf° = -143.177 - 3.772\times10^{-3}T\ln T - 1.837\times10^{-6}T^{2} + 162.400T^{-1} + 93.870\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from King (133). All other data from Stuve (214).

$Re_2O_7(c,1)$

Dirhenium Heptoxide

[Formation: $2Re(c) + 3.5O_2(g) = Re_2O_7(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	39.730	49.540	49.540	0	-301.900	-260.327	190.822
300	39.850	49.785	49.540	.074	-301.893	-260.067	189.456
400	43.903	61.861	51.159	4.281	-301.395	-246.192	134.511
413	44.232	63.270	51.518	4.854	-301.312	-244.399	129.329
413	44.812	63.319	51.518	4.874	-301.292	-244.399	129.329
500	47.894	72.170	54.358	8.906	-300.579	-232.481	101.616
600	51.437	81.215	58.093	13.873	-299.531	-218.957	79.754
600	66.107	107.381	58.093	29.572	-283.832	-218.957	79.754
700	66.107	117.571	65.881	36.183	-281.243	-208.348	65.048

Phase changes: 413 K, α - β transition point of Re_2O_7; $\Delta H°$ = 0.020 kcal/mol.
600 K, melting point of Re_2O_7; $\Delta H°$ = 15.699 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-413 K: $Cp° = 38.437 + 20.618\times10^{-3}T - 4.315\times10^{5}T^{-2}$

$H°- H°_{298} = 38.437\times10^{-3}T + 10.309\times10^{-6}T^2 + 4.315\times10^{2}T^{-1} - 13.824$

413-600 K: $Cp° = 30.181 + 35.426\times10^{-3}T$

$H°- H°_{298} = 30.181\times10^{-3}T + 17.713\times10^{-6}T^2 - 10.612$

600-700 K: $Cp° = 66.101$

$H°- H°_{298} = 66.101\times10^{-3}T - 10.089$

Formation equations (kcal/mol):

298.15-413 K: $\Delta Hf° = -303.976 + 1.780\times10^{-3}T + 7.256\times10^{-6}T^2 + 268.500T^{-1}$

$\Delta Gf° = -303.976 - 1.780\times10^{-3}T\ln T - 7.256\times10^{-6}T^2 + 134.250T^{-1} + 157.196\times10^{-3}T$

413-600 K: $\Delta Hf° = -300.765 - 6.476\times10^{-3}T + 14.660\times10^{-6}T^2 - 163.000T^{-1}$

$\Delta Gf° = -300.765 + 6.476\times10^{-3}T\ln T - 14.660\times10^{-6}T^2 - 81.500T^{-1} + 104.013\times10^{-3}T$

600-700 K: $\Delta Hf° = -300.241 + 29.444\times10^{-3}T - 3.053\times10^{-6}T^2 - 163.000T^{-1}$

$\Delta Gf° = -300.241 - 29.444\times10^{-3}T\ln T + 3.053\times10^{-6}T^2 - 81.500T^{-1} + 322.290\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from King (133). All other data from Stuve (214).

Rh(c,1)

Rhodium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.952	7.542	7.542	0
300	5.958	7.579	7.542	.011
400	6.257	9.335	7.780	.622
500	6.510	10.759	8.237	1.261
600	6.740	11.967	8.762	1.923
700	6.957	13.022	9.296	2.608
800	7.167	13.965	9.821	3.315
900	7.376	14.821	10.330	4.042
1000	7.587	15.609	10.819	4.790
1100	7.805	16.342	11.288	5.559
1200	8.032	17.031	11.739	6.351
1300	8.271	17.683	12.171	7.166
1400	8.528	18.306	12.587	8.006
1500	8.804	18.903	12.988	8.872
1600	9.103	19.481	13.376	9.768
1700	9.429	20.042	13.751	10.694
1800	9.784	20.591	14.117	11.654
1900	10.173	21.130	14.471	12.652
2000	10.597	21.663	14.818	13.690
2100	11.062	22.191	15.156	14.773
2200	11.569	22.717	15.488	15.904
2237	11.769	22.912	15.609	16.336
2237	12.090	25.753	15.609	22.692
2300	12.090	26.089	15.892	23.454
2400	12.090	26.603	16.327	24.663
2500	12.090	27.097	16.748	25.872

Phase change: 2237 K, melting point of Rh; ΔH° = 6.356 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2237 K: $C_p^\circ = 5.046 + 2.654\times10^{-3}T + 0.102\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.046\times10^{-3}T + 1.327\times10^{-6}T^2 - 0.102\times10^{2}T^{-1} - 1.588$

2237-2500 K: $C_p^\circ = 12.090$

$H^\circ - H^\circ_{298} = 12.090\times10^{-3}T - 4.353$

Sources: Low-temperature heat capacities and entropy at 298 K from Furukawa (72). High-temperature data based on Jaeger (102) and Kats (115).

Rh(g)

Rhodium (ideal monatomic gas)

[Formation: Rh(c) = Rh(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	5.022	44.387	44.387	0	133.100	122.115	-89.511
300	5.024	44.418	44.388	.009	133.098	122.046	-88.910
400	5.173	45.882	44.587	.518	132.996	118.377	-64.677
500	5.386	47.058	44.966	1.046	132.885	114.736	-50.150
600	5.617	48.061	45.401	1.596	132.773	111.117	-40.474
700	5.839	48.943	45.844	2.169	132.661	107.516	-33.568
800	6.034	9.736	46.282	2.763	132.548	103.931	-28.392
900	6.198	50.457	46.707	3.375	132.433	100.361	-24.371
1000	6.329	51.117	47.115	4.002	132.312	96.804	-21.156
1100	6.430	51.725	47.507	4.640	132.181	93.260	-18.529
1200	6.505	52.288	47.882	5.287	132.036	89.728	-16.341
1300	6.558	52.811	48.242	5.940	131.874	86.208	-14.493
1400	6.594	53.298	48.585	6.598	131.692	82.703	-12.910
1500	6.616	53.754	48.915	7.258	131.486	79.210	-11.541
1600	6.629	54.181	49.230	7.921	131.253	75.733	-10.345
1700	6.635	54.583	49.534	8.584	130.990	72.270	-9.291
1800	6.636	54.963	49.825	9.248	130.694	68.824	-8.356
1900	6.634	55.321	50.105	9.911	130.359	65.396	-7.522
2000	6.630	55.662	50.375	10.574	129.984	61.986	-6.773

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 5.140 + 1.012\times10^{-3}T - 0.374\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.140\times10^{-3}T + 0.506\times10^{-6}T^2 + 0.374\times10^{2}T^{-1} - 1.703$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 132.985 + 0.094\times10^{-3}T - 0.821\times10^{-6}T^2 + 47.600T^{-1}$

$\Delta Gf^\circ = 132.985 - 0.094\times10^{-3}T\ln T + 0.821\times10^{-6}T^2 + 23.800T^{-1} - 36.437\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). All other data from Hilsenrath (94).

Ru(c,1)

Ruthenium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.730	6.839	6.839	0
300	5.736	6.874	6.839	.011
400	6.041	8.568	7.068	.600
500	6.281	9.943	7.509	1.217
600	6.485	11.107	8.015	1.855
700	6.665	12.120	8.530	2.513
800	6.827	13.021	9.036	3.188
900	6.978	13.834	9.525	3.878
1000	7.122	14.577	9.994	4.583
1100	7.266	15.262	10.442	5.302
1200	7.413	15.901	10.871	6.036
1300	7.567	16.500	11.281	6.785
1400	7.734	17.067	11.674	7.550
1500	7.917	17.606	12.051	8.332
1600	8.121	18.124	12.415	9.134
1700	8.350	18.623	12.766	9.957
1800	8.610	19.107	13.104	10.805
1900	8.903	19.580	13.433	11.680
2000	9.235	20.045	13.752	12.587
2100	9.609	20.505	14.063	13.529
2200	10.030	20.961	14.366	14.510
2300	10.503	21.417	14.662	15.537
2400	11.032	21.875	14.953	16.613
2500	11.620	22.338	15.240	17.745
2600	12.273	22.806	15.522	18.939
2607	12.322	22.839	15.541	19.025
2607	12.400	26.368	15.541	28.225
2700	12.400	26.802	15.921	29.378
2800	12.400	27.253	16.318	30.618
2900	12.400	27.688	16.702	31.858
3000	12.400	28.109	17.076	33.098

Phase change: 2607 K, melting point of Ru; ΔH° = 9.200 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2607 K: $Cp^\circ = 4.707 + 2.408\times10^{-3}T + 0.272\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.707\times10^{-3}T + 1.204\times10^{-6}T^2 - 0.272\times10^{2}T^{-1} - 1.419$

2607-3000 K: $Cp^\circ = 12.400$

$H^\circ - H^\circ_{298} = 12.400\times10^{-3}T - 4.102$

Sources: Low-temperature heat capacities and entropy at 298 K from Furukawa (72). High-temperature data based on Holzmann (96) and Sheindlin (194).

Ru(g)

Ruthenium (ideal monatomic gas)

[Formation: Ru(c,1) = Ru(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	5.144	44.550	44.550	0	153.600	142.356	-104.349
300	5.149	44.582	44.550	.010	153.599	142.287	-103.654
400	5.414	46.099	44.757	.537	153.537	138.525	-75.685
500	5.687	47.337	45.151	1.093	153.476	134.779	-58.911
600	5.918	48.395	45.607	1.673	153.418	131.045	-47.733
700	6.089	49.321	46.072	2.274	153.361	127.320	-39.751
800	6.203	50.142	46.531	2.889	153.301	123.604	-33.767
900	6.268	50.876	46.973	3.513	153.235	119.897	-29.115
1000	6.298	51.539	47.397	4.142	153.159	116.197	-25.395
1100	6.305	52.140	47.802	4.772	153.070	112.504	-22.352
1200	6.301	52.688	48.186	5.402	152.966	108.822	-19.819
1300	6.294	53.192	48.552	6.032	152.847	105.147	-17.677
1400	6.293	53.658	48.900	6.661	152.711	101.484	-15.842
1500	6.300	54.093	49.232	7.291	152.559	97.829	-14.253
1600	6.318	54.500	49.549	7.922	152.388	94.186	-12.865
1700	6.349	54.884	49.852	8.555	152.198	90.554	-11.641
1800	6.392	55.248	50.141	9.192	151.987	86.933	-10.555
1900	6.446	55.595	50.419	9.834	151.754	83.326	-9.584
2000	6.510	55.927	50.686	10.481	151.494	79.730	-8.712
2100	6.581	56.246	50.943	11.136	151.207	76.151	-7.925
2200	6.660	56.554	51.191	11.798	150.888	72.583	-7.210
2300	6.743	56.852	51.431	12.468	150.531	69.031	-6.559
2400	6.829	57.141	51.663	13.147	150.134	65.496	-5.964
2500	6.917	57.421	51.887	13.834	149.689	61.982	-5.418
2600	7.005	57.695	52.107	14.530	149.191	58.480	-4.916
2607	7.011	57.714	52.122	14.579	149.154	58.235	-4.882
2607	7.011	57.714	52.122	14.579	139.954	58.235	-4.882
2700	7.092	57.960	52.317	15.235	139.457	55.330	-4.479
2800	7.178	58.220	52.524	15.948	138.930	52.222	-4.076
2900	7.261	58.473	52.725	16.670	138.412	49.136	-3.703
3000	7.341	58.721	52.921	17.401	137.903	46.067	-3.356

Phase change: 2607 K, melting point of Ru; ΔH° = 9.200 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 5.819 + 0.414\times10^{-3}T - 0.709\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.819\times10^{-3}T + 0.207\times10^{-6}T^2 + 0.709\times10^{2}T^{-1} - 1.991$

Formation equations (kcal/mol):

298.15-2607 K: $\Delta Hf^\circ = 153.028 + 1.112\times10^{-3}T - 0.997\times10^{-6}T^2 + 98.100T^{-1}$

$\Delta Gf^\circ = 153.028 - 1.112\times10^{-3}T\ln T + 0.997\times10^{-6}T^2 + 49.050T^{-1} - 30.306\times10^{-3}T$

2607-3000 K: $\Delta Hf^\circ = 155.711 - 6.581\times10^{-3}T + 0.207\times10^{-6}T^2 + 70.900T^{-1}$

$\Delta Gf^\circ = 155.711 + 6.581\times10^{-3}T\ln T - 0.207\times10^{-6}T^2 + 35.450T^{-1} - 88.707\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). All other data from Hilsenrath (94).

$RuO_2(c)$

Ruthenium Dioxide

[Formation: $Ru(c) + O_2(g) = RuO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.600	13.900	13.900	0	-72.900	-60.394	44.270
300	12.682	13.978	13.900	.024	-72.900	-60.317	43.940
400	15.745	18.112	14.442	1.468	-72.755	-56.137	30.671
500	17.283	21.807	15.555	3.126	-72.445	-52.016	22.736
600	18.246	25.048	16.871	4.906	-72.058	-47.964	17.471
700	18.937	27.915	18.249	6.766	-71.634	-43.983	13.732
800	19.483	30.481	19.621	8.688	-71.185	-40.065	10.945
900	19.945	32.803	20.959	10.660	-70.717	-36.202	8.791
1000	20.355	34.926	22.251	12.675	-70.234	-32.393	7.079
1100	20.730	36.884	23.493	14.730	-69.737	-28.632	5.689
1200	21.083	38.703	24.685	16.821	-69.228	-24.917	4.538

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 18.315 + 2.586\times10^{-3}T - 5.765\times10^{5}T^{-2}$

$H°- H°_{298} = 18.315\times10^{-3}T + 1.293\times10^{-6}T^{2} + 5.765\times10^{2}T^{-1} - 7.509$

Formation equations (kcal/mol):

298.15-1200 K: $\Delta Hf° = -76.638 + 6.378\times10^{-3}T - 0.414\times10^{-6}T^{2} + 558.500T^{-1}$

$\Delta Gf° = -76.638 - 6.378\times10^{-3}T\ln T + 0.414\times10^{-6}T^{2} + 279.250T^{-1} + 87.556\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). Entropy at 298 K from Chatterji (34). High-temperature data based on Fredrickson (69).

S(c,l)

Sulfur

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.425	7.661	7.661	0
300	5.436	7.695	7.662	.010
368.3	5.795	8.846	7.776	.394
368.3	5.921	9.106	7.776	.490
388.36	6.015	9.423	7.854	.609
388.36	7.423	10.486	7.854	1.022
400	7.687	10.709	7.934	1.110
432.02	12.860	11.340	8.162	1.373
500	9.078	12.797	8.703	2.047
600	8.200	14.362	9.522	2.904
700	7.799	15.596	10.305	3.704
717.824	7.694	15.790	10.439	3.841

Phase changes: 368.3 K, orthorhombic - monoclinic transformation of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-368.3 K: $Cp^\circ = 8.174 - 3.434\times10^{-3}T - 1.556\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.174\times10^{-3}T - 1.717\times10^{-6}T^2 + 1.556\times10^{2}T^{-1} - 2.806$

368.3-388.36 K: $Cp^\circ = 5.911 + 0.058\times10^{-3}T$

$H^\circ - H^\circ_{298} = 5.911\times10^{-3}T + 0.029\times10^{-6}T^2 - 1.691$

388.36-432.02 K: $Cp^\circ = -38.829 + 86.622\times10^{-3}T + 19.022\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = -38.829\times10^{-3}T + 43.311\times10^{-6}T^2 - 19.022\times10^{2}T^{-1} + 14.467$

432.02-717.824 K: $Cp^\circ = -34.923 + 46.998\times10^{-3}T + 51.287\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = -34.923\times10^{-3}T + 23.499\times10^{-6}T^2 - 51.287\times10^{2}T^{-1} + 23.946$

Sources: Data based on Montgomery (159) and West (243).

S(g)

Sulfur (ideal monatomic gas)

[Reaction: $0.5S_2(g) = S(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.658	40.086	40.086	0	50.845	47.019	-34.465
300	5.657	40.121	40.088	.010	50.848	46.995	-34.235
400	5.553	41.735	40.307	.571	51.010	45.685	-24.961
500	5.435	42.961	40.719	1.121	51.146	44.339	-19.380
600	5.339	43.943	41.178	1.659	51.260	42.965	-15.650
700	5.266	44.761	41.634	2.189	51.360	41.574	-12.980
800	5.210	45.460	42.069	2.713	51.448	40.171	-10.974
900	5.168	46.071	42.480	3.232	51.528	38.757	-9.411
1000	5.136	46.614	42.867	3.747	51.599	37.333	-8.159
1100	5.111	47.102	43.230	4.259	51.664	35.904	-7.133
1200	5.093	47.546	43.572	4.769	51.722	34.468	-6.277
1300	5.079	47.953	43.893	5.278	51.777	33.028	-5.553
1400	5.069	48.329	44.197	5.785	51.826	31.584	-4.930
1500	5.064	48.679	44.484	6.292	51.870	30.136	-4.391
1600	5.062	49.005	44.756	6.798	51.911	28.687	-3.918
1700	5.063	49.312	45.016	7.304	51.947	27.234	-3.501
1800	5.068	49.602	45.263	7.811	51.982	25.779	-3.130
1900	5.075	49.876	45.498	8.318	52.014	24.322	-2.798
2000	5.085	50.137	45.724	8.826	52.044	22.864	-2.498
2100	5.097	50.385	45.940	9.335	52.071	21.404	-2.228
2200	5.111	50.622	46.147	9.845	52.098	19.944	-1.981
2300	5.127	50.850	46.347	10.357	52.125	18.481	-1.756
2400	5.144	51.068	46.538	10.871	52.151	17.019	-1.550
2500	5.162	51.279	46.725	11.386	52.176	15.554	-1.360
2600	5.181	51.482	46.904	11.903	52.201	14.087	-1.184
2700	5.200	51.678	47.077	12.422	52.228	12.620	-1.022
2800	5.219	51.867	47.244	12.943	52.254	11.155	-.871
2900	5.239	52.050	47.407	13.466	52.282	9.688	-.730
3000	5.258	52.228	47.564	13.991	52.310	8.218	-.599

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 5.397 - 0.226\times10^{-3}T + 0.292\times10^{5}T^{-2}$

$H°- H°_{298} = 5.397\times10^{-3}T - 0.113\times10^{-6}T^{2} - 0.292\times10^{2}T^{-1} - 1.501$

2000-3000 K: $Cp° = 4.156 + 0.336\times10^{-3}T + 10.352\times10^{5}T^{-2}$

$H°- H°_{298} = 4.156\times10^{-3}T + 0.168\times10^{-6}T^{2} - 10.352\times10^{2}T^{-1} + 0.360$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H° = 50.716 + 1.225\times10^{-3}T - 0.273\times10^{-6}T^{2} - 63.350T^{-1}$

$\Delta G° = 50.716 - 1.225\times10^{-3}T\ln T + 0.273\times10^{-6}T^{2} - 31.675T^{-1} - 5.144\times10^{-3}T$

2000-3000 K: $\Delta H° = 53.602 - 0.599\times10^{-3}T + 0.118\times10^{-6}T^{2} - 1665.200T^{-1}$

$\Delta G° = 53.602 + 0.599\times10^{-3}T\ln T - 0.118\times10^{-6}T^{2} - 832.600T^{-1} - 19.473\times10^{-3}T$

Source: Data from JANAF (54).

$S_2(g)$

Sulfur (ideal diatomic gas)

[Formation: $2S(c,l) = S_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.765	54.506	54.506	0	30.710	19.027	-13.947
300	7.774	54.555	54.508	.014	30.704	18.954	-13.808
368.3	8.029	56.177	54.669	.556	30.478	16.304	-9.674
368.3	8.029	56.177	54.669	.556	30.286	16.304	-9.674
388.36	8.104	56.605	54.758	.717	30.209	15.545	-8.748
388.36	8.104	56.605	54.758	.717	29.383	15.545	-8.748
400	8.148	56.845	54.815	.812	29.302	15.131	-8.267
432.02	8.226	57.475	54.989	1.074	29.038	14.006	-7.085
500	8.392	58.691	55.413	1.639	28.255	11.706	-5.117
600	8.553	60.236	56.091	2.487	27.389	8.482	-3.089
700	8.666	61.563	56.780	3.348	26.650	5.390	-1.683
717.824	8.682	61.781	56.902	3.503	26.531	4.852	-1.477

Phase changes: 368.3 K, orthorhombic - monoclinic transformation of S; $\Delta H°$ = 0.096 kcal/mol.
388.36 K, melting point of S; $\Delta H°$ = 0.413 kcal/mol.
432.02 K, second order transformation of S; $\Delta H°$ = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.343 + 0.640\times10^{-3}T - 0.683\times10^{5}T^{-2}$

$H°- H°_{298} = 8.343\times10^{-3}T + 0.320\times10^{-6}T^{2} + 0.683\times10^{2}T^{-1} - 2.745$

2000-3000 K: $Cp° = 9.510 + 0.200\times10^{-3}T - 12.600\times10^{5}T^{-2}$

$H°- H°_{298} = 9.510\times10^{-3}T + 0.100\times10^{-6}T^{2} + 12.600\times10^{2}T^{-1} - 4.795$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta Hf° = 33.578 - 8.005\times10^{-3}T + 3.754\times10^{-6}T^{2} - 242.900T^{-1}$

$\Delta Gf° = 33.578 + 8.005\times10^{-3}T\ln T - 3.754\times10^{-6}T^{2} - 121.450T^{-1} - 91.926\times10^{-3}T$

368.3-388.36 K: $\Delta Hf° = 31.347 - 3.479\times10^{-3}T + 0.262\times10^{-6}T^{2} + 68.300T^{-1}$

$\Delta Gf° = 31.347 + 3.479\times10^{-3}T\ln T - 0.262\times10^{-6}T^{2} + 34.150T^{-1} - 61.560\times10^{-3}T$

388.36-432.02 K: $\Delta Hf° = -0.969 + 86.001\times10^{-3}T - 86.302\times10^{-6}T^{2} + 3872.700T^{-1}$

$\Delta Gf° = -0.969 - 86.001\times10^{-3}T\ln T + 86.302\times10^{-6}T^{2} + 1936.350T^{-1} + 508.897\times10^{-3}T$

432.02-717.824 K: $\Delta Hf° = -19.927 + 78.189\times10^{-3}T - 46.678\times10^{-6}T^{2} + 10325.700T^{-1}$

$\Delta Gf° = -19.927 - 78.189\times10^{-3}T\ln T + 46.678\times10^{-6}T^{2} + 5162.850T^{-1} + 505.202\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (36). All other data from JANAF (54).

$S_2(g)$

Sulfur (ideal diatomic gas)

T, K	cal/mol•K			$H°- H°_{298}$,
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	kcal/mol
298.15	7.765	54.506	54.506	0
300	7.774	54.555	54.508	.014
400	8.148	56.845	54.815	.812
500	8.392	58.691	55.413	1.639
600	8.553	60.236	56.091	2.487
700	8.666	61.563	56.780	3.348
800	8.756	62.727	57.453	4.219
900	8.835	63.762	58.096	5.099
1000	8.909	64.697	58.711	5.986
1100	8.983	65.550	59.295	6.881
1200	9.057	66.335	59.849	7.783
1300	9.131	67.062	60.376	8.692
1400	9.205	67.742	60.878	9.609
1500	9.278	68.379	61.357	10.533
1600	9.348	68.980	61.815	11.464
1700	9.415	69.549	62.253	12.403
1800	9.479	70.089	62.674	13.347
1900	9.539	70.603	63.078	14.298
2000	9.595	71.094	63.467	15.255
2100	9.644	71.563	63.841	16.217
2200	9.691	72.013	64.202	17.184
2300	9.734	72.445	64.552	18.155
2400	9.775	72.860	64.889	19.131
2500	9.812	73.260	65.216	20.110
2600	9.842	73.645	65.532	21.093
2700	9.871	74.017	65.840	22.078
2800	9.898	74.377	66.139	23.067
2900	9.924	74.725	66.429	24.058
3000	9.949	75.061	66.711	25.051

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.343 + 0.640\times10^{-3}T - 0.683\times10^{5}T^{-2}$

$H°- H°_{298} = 8.343\times10^{-3}T + 0.320\times10^{-6}T^{2} + 0.683\times10^{2}T^{-1} - 2.745$

2000-3000 K: $Cp° = 9.510 + 0.200\times10^{-3}T - 12.600\times10^{5}T^{-2}$

$H°- H°_{298} = 9.510\times10^{-3}T + 0.100\times10^{-6}T^{2} + 12.600\times10^{2}T^{-1} - 4.795$

Source: Data from JANAF (54).

$S_3(g)$

Sulfur (ideal triatomic gas)

[Reaction: $1.5S_2(g) = S_3(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	11.493	65.275	65.275	0	-11.793	-6.878	5.042
300	11.514	65.346	65.276	.021	-11.793	-6.847	4.988
400	12.354	68.785	65.740	1.218	-11.793	-5.200	2.841
500	12.840	71.599	66.639	2.480	-11.771	-3.553	1.553
600	13.137	73.968	67.668	3.780	-11.743	-1.912	.696
700	13.327	76.008	68.717	5.104	-11.711	-.275	.086
800	13.457	77.797	69.742	6.444	-11.678	1.357	-.371
900	13.548	79.387	70.727	7.794	-11.647	2.983	-.724
1000	13.614	80.818	71.666	9.152	-11.620	4.608	-1.007
1100	13.664	82.118	72.557	10.517	-11.597	6.230	-1.238
1200	13.702	83.309	73.405	11.885	-11.583	7.850	-1.430
1300	13.733	84.407	74.209	13.257	-11.574	9.468	-1.592
1400	13.757	85.425	74.974	14.631	-11.576	11.088	-1.731
1500	13.776	86.375	75.703	16.008	-11.585	12.706	-1.851
1600	13.792	87.265	76.399	17.386	-11.603	14.325	-1.957
1700	13.806	88.101	77.062	18.766	-11.632	15.947	-2.050
1800	13.817	88.891	77.698	20.148	-11.666	17.571	-2.133
1900	13.826	89.638	78.307	21.529	-11.711	19.195	-2.208
2000	13.834	90.348	78.892	22.913	-11.763	20.824	-2.275
2100	13.841	91.023	79.453	24.296	-11.822	22.453	-2.337
2200	13.848	91.667	79.994	25.681	-11.888	24.087	-2.393
2300	13.853	92.283	80.515	27.066	-11.959	25.725	-2.444
2400	13.857	92.872	81.017	28.451	-12.038	27.365	-2.492
2500	13.862	93.438	81.503	29.837	-12.121	29.009	-2.536
2600	13.865	93.982	81.973	31.224	-12.209	30.654	-2.577
2700	13.869	94.505	82.427	32.610	-12.300	32.305	-2.615
2800	13.871	95.009	82.867	33.997	-12.396	33.962	-2.651
2900	13.874	95.496	83.294	35.385	-12.495	35.620	-2.684
3000	13.876	95.967	83.710	36.772	-12.598	37.276	-2.716

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 13.561 + 0.170\times10^{-3}T - 1.883\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.561\times10^{-3}T + 0.085\times10^{-6}T^2 + 1.883\times10^{2}T^{-1} - 4.682$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = -12.358 + 1.046\times10^{-3}T - 0.395\times10^{-6}T^2 + 85.850T^{-1}$

$\Delta G^\circ = -12.358 - 1.046\times10^{-3}T\ln T + 0.395\times10^{-6}T^2 + 42.925T^{-1} + 23.740\times10^{-3}T$

2000-3000 K: $\Delta H^\circ = -9.283 - 0.704\times10^{-3}T - 0.065\times10^{-6}T^2 - 1701.700T^{-1}$

$\Delta G^\circ = -9.283 + 0.704\times10^{-3}T\ln T + 0.065\times10^{-6}T^2 - 850.850T^{-1} + 9.781\times10^{-3}T$

Source: Data from Gurvich (91).

$S_4(g)$

Sulfur (ideal tetratomic gas)

[Reaction: $2S_2(g) = S_4(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	15.761	70.128	70.128	0	-29.003	-17.410	12.762
300	15.796	70.226	70.129	.029	-29.002	-17.337	12.630
400	17.225	74.985	70.768	1.687	-28.940	-13.458	7.353
500	18.050	78.925	72.017	3.454	-28.827	-9.598	4.195
600	18.553	82.264	73.454	5.286	-28.691	-5.766	2.100
700	18.877	85.150	74.923	7.159	-28.540	-1.957	.611
800	19.097	87.686	76.363	9.058	-28.383	1.831	-.500
900	19.253	89.945	77.749	10.976	-28.225	5.596	-1.359
1000	19.366	91.980	79.072	12.908	-28.067	9.347	-2.043
1100	19.451	93.829	80.330	14.849	-27.916	13.082	-2.599
1200	19.517	95.525	81.528	16.797	-27.772	16.802	-3.060
1300	19.568	97.089	82.665	18.751	-27.636	20.509	-3.448
1400	19.609	98.541	83.748	20.710	-27.511	24.209	-3.779
1500	19.642	99.895	84.780	22.673	-27.396	27.898	-4.065
1600	19.670	101.163	85.764	24.639	-27.292	31.583	-4.314
1700	19.693	102.357	86.706	26.607	-27.202	35.258	-4.533
1800	19.712	103.483	87.607	28.577	-27.120	38.931	-4.727
1900	19.728	104.549	88.471	30.549	-27.050	42.598	-4.900
2000	19.742	105.561	89.299	32.523	-26.990	46.264	-5.055
2100	19.754	106.525	90.098	34.497	-26.940	49.922	-5.195
2200	19.764	107.444	90.865	36.473	-26.898	53.582	-5.323
2300	19.773	108.323	91.606	38.450	-26.863	57.241	-5.439
2400	19.781	109.164	92.319	40.428	-26.837	60.897	-5.545
2500	19.789	109.972	93.010	42.406	-26.817	64.553	-5.643
2600	19.795	110.748	93.676	44.386	-26.803	68.206	-5.733
2700	19.800	111.495	94.323	46.365	-26.794	71.861	-5.817
2800	19.805	112.216	94.950	48.346	-26.791	75.515	-5.894
2900	19.810	112.911	95.557	50.326	-26.793	79.170	-5.966
3000	19.814	113.582	96.146	52.308	-26.797	82.823	-6.034

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 19.279 + 0.288\times10^{-3}T - 3.204\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.279\times10^{-3}T + 0.144\times10^{-6}T^2 + 3.204\times10^{2}T^{-1} - 6.835$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = -30.348 + 2.593\times10^{-3}T - 0.496\times10^{-6}T^2 + 183.800T^{-1}$

$\Delta G^\circ = -30.348 - 2.593\times10^{-3}T\ln T + 0.496\times10^{-6}T^2 + 91.900T^{-1} + 56.989\times10^{-3}T$

2000-3000 K: $\Delta H^\circ = -26.249 + 0.259\times10^{-3}T - 0.056\times10^{-6}T^2 - 2199.600T^{-1}$

$\Delta G^\circ = -26.249 - 0.259\times10^{-3}T\ln T + 0.056\times10^{-6}T^2 - 1099.800T^{-1} + 38.376\times10^{-3}T$

Source: Data from Gurvich (91).

$S_5(g)$

Sulfur (ideal pentatomic gas)

[Reaction: $2.5S_2(g) = S_5(g)$]

T, K	cal/mol•K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	21.331	80.629	80.629	0	-47.071	-30.483	22.344
300	21.373	80.761	80.629	.040	-47.066	-30.378	22.130
400	23.035	87.163	81.491	2.269	-46.832	-24.852	13.578
500	23.941	92.410	83.166	4.622	-46.546	-19.388	8.474
600	24.478	96.826	85.084	7.045	-46.243	-13.985	5.094
700	31.272	100.627	87.040	9.511	-45.930	-8.634	2.696
800	25.046	103.957	88.951	12.005	-45.614	-3.325	.908
900	25.206	106.917	90.786	14.518	-45.300	1.939	-.471
1000	25.322	109.579	92.534	17.045	-44.991	7.172	-1.568
1100	25.409	111.996	94.194	19.582	-44.691	12.375	-2.459
1200	25.475	114.210	95.772	22.126	-44.402	17.550	-3.196
1300	25.528	116.251	97.269	24.676	-44.125	22.700	-3.816
1400	25.569	118.145	98.694	27.231	-43.862	27.831	-4.345
1500	25.603	119.910	100.050	29.790	-43.613	32.943	-4.800
1600	25.630	121.563	101.344	32.351	-43.380	38.039	-5.196
1700	25.653	123.118	102.579	34.916	-43.162	43.120	-5.543
1800	25.673	124.585	103.762	37.482	-42.957	48.191	-5.851
1900	25.689	125.973	104.894	40.050	-42.766	53.250	-6.125
2000	25.703	127.291	105.981	42.620	-42.589	58.299	-6.371
2100	25.715	128.546	107.026	45.191	-42.422	63.337	-6.591
2200	25.725	129.742	108.032	47.763	-42.268	68.371	-6.792
2300	25.735	130.886	109.001	50.336	-42.123	73.398	-6.974
2400	25.743	131.981	109.936	52.909	-41.990	78.416	-7.141
2500	25.750	133.032	110.838	55.484	-41.862	83.433	-7.294
2600	25.756	134.042	111.712	58.059	-41.745	88.439	-7.434
2700	25.762	135.015	112.558	60.635	-41.631	93.443	-7.564
2800	25.767	135.951	113.375	63.212	-41.527	98.450	-7.684
2900	25.771	136.856	114.170	65.789	-41.427	103.447	-7.796
3000	25.775	137.729	114.940	68.366	-41.333	108.438	-7.900

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 25.297 + 0.306\times10^{-3}T - 3.607\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.297\times10^{-3}T + 0.153\times10^{-6}T^2 + 3.607\times10^{2}T^{-1} - 8.766$

2000-3000 K: $Cp^\circ = 26.003 - 0.050\times10^{-3}T - 7.986\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 26.003\times10^{-3}T - 0.025\times10^{-6}T^2 + 7.986\times10^{2}T^{-1} - 9.685$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = -48.974 + 4.439\times10^{-3}T - 0.647\times10^{-6}T^2 + 189.950T^{-1}$

$\Delta G^\circ = -48.974 - 4.439\times10^{-3}T\ln T + 0.647\times10^{-6}T^2 + 94.975T^{-1} + 86.053\times10^{-3}T$

2000-3000 K: $\Delta H^\circ = -44.769 + 2.228\times10^{-3}T - 0.275\times10^{-6}T^2 - 2351.400T^{-1}$

$\Delta G^\circ = -44.769 - 2.228\times10^{-3}T\ln T + 0.275\times10^{-6}T^2 - 1175.700T^{-1} + 68.202\times10^{-3}T$

Source: Data from Gurvich (91).

$S_6(g)$

Sulfur (ideal hexatomic gas)

[Reaction: $3S_2(g) = S_6(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta H°$	$\Delta G°$	
298.15	26.901	84.555	84.555	0	-68.126	-44.583	32.680
300	26.951	84.721	84.555	.050	-68.118	-44.435	32.370
400	28.846	92.766	85.638	2.851	-67.711	-36.603	19.999
500	29.834	99.319	87.741	5.789	-67.254	-28.877	12.622
600	30.403	104.813	90.140	8.804	-66.783	-21.246	7.739
700	30.759	109.529	92.582	11.863	-66.307	-13.695	4.276
800	30.995	113.652	94.962	14.952	-65.831	-6.208	1.696
900	31.159	117.313	97.246	18.060	-65.363	1.213	-.294
1000	31.278	120.603	99.421	21.182	-64.902	8.586	-1.876
1100	31.366	123.588	101.484	24.314	-64.455	15.913	-3.162
1200	31.434	126.321	103.442	27.455	-64.020	23.201	-4.225
1300	31.487	128.839	105.300	30.601	-63.601	30.450	-5.119
1400	31.529	131.174	107.066	33.751	-63.202	37.671	-5.881
1500	31.563	133.350	108.746	36.906	-62.819	44.861	-6.536
1600	31.591	135.388	110.348	40.064	-62.454	52.029	-7.107
1700	31.614	137.304	111.878	43.224	-62.111	59.172	-7.607
1800	31.633	139.112	113.341	46.387	-61.780	66.299	-8.050
1900	31.650	140.822	114.743	49.551	-61.469	73.406	-8.444
2000	31.664	142.446	116.088	52.717	-61.174	80.498	-8.796
2100	31.676	143.991	117.380	55.883	-60.894	87.572	-9.114
2200	31.687	145.465	118.623	59.052	-60.626	94.637	-9.401
2300	31.696	146.874	119.821	62.221	-60.370	101.690	-9.663
2400	31.704	148.223	120.977	65.391	-60.128	108.729	-9.901
2500	31.711	149.517	122.093	68.561	-59.895	115.763	-10.120
2600	31.718	150.761	123.171	71.733	-59.672	122.780	-10.320
2700	31.723	151.958	124.215	74.905	-59.455	129.796	-10.506
2800	31.728	153.112	125.227	78.077	-59.250	136.803	-10.678
2900	31.733	154.226	126.208	81.251	-59.049	143.803	-10.837
3000	31.737	155.301	127.160	84.424	-58.855	150.791	-10.985

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 31.351 + 0.262\times10^{-3}T - 4.027\times10^{5}T^{-2}$

$H°- H°_{298} = 31.351\times10^{-3}T + 0.131\times10^{-6}T^{2} + 4.027\times10^{2}T^{-1} - 10.710$

2000-3000 K: $Cp° = 29.750 + 0.600\times10^{-3}T + 28.557\times10^{5}T^{-2}$

$H°- H°_{298} = 29.750\times10^{-3}T + 0.300\times10^{-6}T^{2} - 28.557\times10^{5}T^{-1} - 6.555$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H° = -70.601 + 6.322\times10^{-3}T - 0.829\times10^{-6}T^{2} + 197.800T^{-1}$

$\Delta G° = -70.601 - 6.322\times10^{-3}T\ln T + 0.829\times10^{-6}T^{2} + 98.900T^{-1} + 121.923\times10^{-3}T$

2000-3000 K: $\Delta H° = -60.296 + 1.220\times10^{-3}T - 6635.700T^{-1}$

$\Delta G° = -60.296 - 1.220\times10^{-3}T\ln T - 3317.850T^{-1} + 80.503\times10^{-3}T$

Source: Data from Gurvich (91).

$S_7(g)$

Sulfur (ideal heptatomic gas)

[Reaction: $3.5S_2(g) = S_7(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	31.990	95.508	95.508	0	-81.816	-53.413	39.153
300	32.049	95.706	95.509	.059	-81.806	-53.235	38.781
400	34.276	105.268	96.798	3.388	-81.270	-43.794	23.928
500	35.440	113.054	99.294	6.880	-80.673	-34.490	15.075
600	36.112	119.580	102.147	10.460	-80.061	-25.313	9.220
700	36.532	125.181	105.047	14.094	-79.440	-16.237	5.069
800	36.811	130.078	107.876	17.762	-78.821	-7.247	1.980
900	37.005	134.426	110.589	21.453	-78.209	1.657	-.402
1000	37.145	138.332	113.171	25.161	-77.606	10.501	-2.295
1100	37.249	141.878	115.623	28.881	-77.018	19.283	-3.831
1200	37.329	145.122	117.947	32.610	-76.446	28.014	-5.102
1300	37.392	148.113	120.155	36.346	-75.892	36.693	-6.169
1400	37.441	150.886	122.252	40.088	-75.359	45.336	-7.077
1500	37.482	153.470	124.247	43.834	-74.847	53.937	-7.859
1600	37.515	155.890	126.150	47.584	-74.356	62.508	-8.538
1700	37.542	158.166	127.968	51.337	-73.889	71.045	-9.133
1800	37.565	160.312	129.705	55.093	-73.437	79.562	-9.660
1900	37.585	162.344	131.370	58.850	-73.009	88.047	-10.128
2000	37.602	164.272	132.967	62.610	-72.599	96.516	-10.547
2100	37.616	166.107	134.502	66.370	-72.205	104.958	-10.923
2200	37.628	167.857	135.979	70.132	-71.828	113.387	-11.264
2300	37.639	169.530	137.401	73.896	-71.463	121.801	-11.574
2400	37.649	171.132	138.774	77.660	-71.114	130.193	-11.856
2500	37.657	172.669	140.099	81.426	-70.775	138.577	-12.114
2600	37.665	174.146	141.380	85.192	-70.450	146.940	-12.351
2700	37.671	175.568	142.621	88.958	-70.131	155.296	-12.570
2800	37.677	176.938	143.822	92.726	-69.825	163.644	-12.773
2900	37.683	178.260	144.986	96.494	-69.525	171.980	-12.961
3000	37.688	179.538	146.117	100.262	-69.233	180.294	-13.134

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 37.220 + 0.316\times10^{-3}T - 4.734\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 37.220\times10^{-3}T + 0.158\times10^{-6}T^2 + 4.734\times10^{2}T^{-1} - 12.699$

2000-3000 K: $Cp^\circ = 37.582 + 0.050\times10^{-3}T - 3.218\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 37.582\times10^{-3}T + 0.025\times10^{-6}T^2 + 3.218\times10^{2}T^{-1} - 12.815$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = -84.908 + 8.019\times10^{-3}T - 0.962\times10^{-6}T^2 + 234.350T^{-1}$

$\Delta G^\circ = -84.908 - 8.019\times10^{-3}T\ln T + 0.962\times10^{-6}T^2 + 117.175T^{-1} + 149.719\times10^{-3}T$

2000-3000 K: $\Delta H^\circ = -77.849 + 4.297\times10^{-3}T - 0.325\times10^{-6}T^2 - 4088.200T^{-1}$

$\Delta G^\circ = -77.849 - 4.297\times10^{-3}T\ln T + 0.325\times10^{-6}T^2 - 2044.100T^{-1} + 119.710\times10^{-3}T$

Source: Data from Gurvich (91).

$S_8(g)$

Sulfur (ideal octatomic gas)

[Reaction: $4S_2(g) = S_8(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	37.186	101.741	101.741	0	-98.959	-64.289	47.125
300	37.251	101.971	101.741	.069	-98.946	-64.071	46.675
400	39.761	113.073	103.238	3.934	-98.273	-52.550	28.712
500	41.080	122.101	106.137	7.982	-97.533	-41.201	18.009
600	41.844	129.664	109.444	12.132	-96.775	-30.007	10.930
700	42.322	136.153	112.807	16.342	-96.009	-18.940	5.913
800	42.639	141.826	116.087	20.591	-95.244	-7.978	2.180
900	42.860	146.862	119.233	24.866	-94.489	2.878	-.699
1000	43.020	151.386	122.225	29.161	-93.742	13.660	-2.985
1100	43.139	155.492	125.066	33.469	-93.014	24.365	-4.841
1200	43.230	159.250	127.760	37.788	-92.303	35.005	-6.375
1300	43.302	162.713	130.318	42.114	-91.613	45.582	-7.663
1400	43.359	165.924	132.748	46.447	-90.948	56.114	-8.760
1500	43.404	168.918	135.061	50.786	-90.305	66.592	-9.702
1600	43.442	171.720	137.265	55.128	-89.687	77.033	-10.522
1700	43.474	174.355	139.370	59.474	-89.097	87.433	-11.240
1800	43.500	176.840	141.383	63.822	-88.525	97.804	-11.875
1900	43.522	179.193	143.312	68.174	-87.977	108.139	-12.439
2000	43.541	181.426	145.162	72.527	-87.452	118.448	-12.943
2100	43.557	183.550	146.940	76.882	-86.945	128.729	-13.397
2200	43.572	185.577	148.651	81.238	-86.457	138.988	-13.807
2300	43.584	187.514	150.298	85.596	-85.983	149.229	-14.180
2400	43.595	189.369	151.888	89.955	-85.528	159.442	-14.519
2500	43.605	191.149	153.423	94.315	-85.084	169.644	-14.830
2600	43.613	192.859	154.907	98.676	-84.655	179.820	-15.115
2700	43.621	194.506	156.344	103.038	-84.233	189.984	-15.378
2800	43.628	196.092	157.735	107.400	-83.827	200.138	-15.621
2900	43.634	197.623	159.084	111.763	-83.428	210.275	-15.847
3000	43.639	199.103	160.394	116.127	-83.036	220.387	-16.055

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 43.137 + 0.332\times10^{-3}T - 5.378\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 43.137\times10^{-3}T + 0.166\times10^{-6}T^2 + 5.378\times10^{2}T^{-1} - 14.680$

2000-3000 K: $Cp^\circ = 43.703 + 0.004\times10^{-3}T - 6.801\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 43.703\times10^{-3}T + 0.002\times10^{-6}T^2 + 6.801\times10^{2}T^{-1} - 15.227$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = -102.659 + 9.765\times10^{-3}T - 1.114\times10^{-6}T^2 + 264.600T^{-1}$

$\Delta G^\circ = -102.659 - 9.765\times10^{-3}T\ln T + 1.114\times10^{-6}T^2 + 132.300T^{-1} + 182.509\times10^{-3}T$

2000-3000 K: $\Delta H^\circ = -95.007 + 5.663\times10^{-3}T - 0.398\times10^{-6}T^2 - 4359.900T^{-1}$

$\Delta G^\circ = -95.007 - 5.663\times10^{-3}T\ln T + 0.398\times10^{-6}T^2 - 2179.950T^{-1} + 149.514\times10^{-3}T$

Source: Data from Gurvich (91).

SO(g)

Sulfur Oxide (ideal gas)

[Formation: $S(c,1) + 0.5O_2(g) = SO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.212	53.020	53.020	0	1.200	-5.018	3.679
300	7.217	53.064	53.021	.013	1.197	-5.057	3.684
368.3	7.440	54.566	53.172	.514	1.072	-6.468	3.838
368.3	7.440	54.566	53.172	.514	.976	-6.468	3.838
388.36	7.505	54.963	53.255	.663	.935	-6.872	3.867
388.36	7.505	54.963	53.255	.663	.522	-6.872	3.867
400	7.543	55.185	53.308	.751	.480	-7.093	3.875
432.02	7.640	55.770	53.469	.994	.344	-7.694	3.892
500	7.846	56.901	53.859	1.521	-.053	-8.925	3.901
600	8.087	58.354	54.491	2.318	-.490	-10.657	3.882
700	8.273	59.615	55.134	3.137	-.860	-12.320	3.846
717.824	8.298	59.823	55.247	3.285	-.920	-12.611	3.839

Phase changes: 368.3 K, orthorhombic-monoclinic transformation of S; $\Delta H° = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H° = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H° = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:
$$Cp° = 7.857 + 0.754\times10^{-3}T - 0.773\times10^{5}T^{-2}$$
$$H°- H°_{298} = 7.857\times10^{-3}T + 0.377\times10^{-6}T^{2} + 0.773\times10^{2}T^{-1} - 2.635$$

2000-3000 K:
$$Cp° = 8.917 + 0.318\times10^{-3}T - 11.935\times10^{5}T^{-2}$$
$$H°- H°_{298} = 8.917\times10^{-3}T + 0.159\times10^{-6}T^{2} + 11.935\times10^{2}T^{-1} - 4.441$$

Formation equations (kcal/mol):

298.15-368.3 K:
$$\Delta Hf° = 2.547 - 3.932\times10^{-3}T + 1.843\times10^{-6}T^{2} - 100.900T^{-1}$$
$$\Delta Gf° = 2.547 + 3.932\times10^{-3}T\ln T - 1.843\times10^{-6}T^{2} - 50.450T^{-1} - 46.660\times10^{-3}T$$

368.3-388.36 K:
$$\Delta Hf° = 1.432 - 1.669\times10^{-3}T + 0.097\times10^{-6}T^{2} + 54.700T^{-1}$$
$$\Delta Gf° = 1.432 + 1.669\times10^{-3}T\ln T - 0.097\times10^{-6}T^{2} + 27.350T^{-1} - 31.477\times10^{-3}T$$

388.36-432.02 K:
$$\Delta Hf° = -14.726 + 43.071\times10^{-3}T - 43.186\times10^{-6}T^{2} + 1956.900T^{-1}$$
$$\Delta Gf° = -14.726 - 43.071\times10^{-3}T\ln T + 43.186\times10^{-6}T^{2} + 978.450T^{-1} + 253.751\times10^{-3}T$$

432.02-717.824 K:
$$\Delta Hf° = -24.205 + 39.165\times10^{-3}T - 23.374\times10^{-6}T^{2} + 5183.400T^{-1}$$
$$\Delta Gf° = -24.205 - 39.165\times10^{-3}T\ln T + 23.374\times10^{-6}T^{2} + 2591.700T^{-1} + 251.904\times10^{-3}T$$

Source: Data from JANAF (53).

SO(g)

Sulfur Oxide (ideal gas)

[Reaction: $0.5S_2(g) + 0.5O_2(g) = SO(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	7.212	53.020	53.020	0	-14.155	-14.532	10.652
300	7.217	53.064	53.021	.013	-14.155	-14.534	10.588
400	7.543	55.185	53.308	.751	-14.171	-14.658	8.009
500	7.846	56.901	53.859	1.521	-14.180	-14.778	6.459
600	8.087	58.354	54.491	2.318	-14.185	-14.897	5.426
700	8.273	59.615	55.134	3.137	-14.185	-15.015	4.688
800	8.414	60.730	55.766	3.971	-14.186	-15.135	4.135
900	8.526	61.727	56.373	4.819	-14.185	-15.253	3.704
1000	8.617	62.631	56.955	5.676	-14.185	-15.372	3.360
1100	8.695	63.456	57.510	6.541	-14.187	-15.492	3.078
1200	8.765	64.215	58.037	7.414	-14.189	-15.609	2.843
1300	8.830	64.919	58.539	8.294	-14.192	-15.727	2.644
1400	8.893	65.576	59.019	9.180	-14.196	-15.846	2.474
1500	8.955	66.192	59.477	10.073	-14.200	-15.964	2.326
1600	9.017	66.772	59.915	10.971	-14.206	-16.082	2.197
1700	9.077	67.320	60.334	11.876	-14.212	-16.198	2.082
1800	9.138	67.841	60.737	12.787	-14.217	-16.314	1.981
1900	9.197	68.336	61.123	13.704	-14.222	-16.430	1.890
2000	9.256	68.810	61.497	14.626	-14.228	-16.548	1.808
2100	9.313	69.263	61.856	15.555	-14.232	-16.663	1.734
2200	9.369	69.697	62.202	16.489	-14.237	-16.778	1.667
2300	9.423	70.115	62.537	17.429	-14.241	-16.894	1.605
2400	9.474	70.517	62.862	18.373	-14.245	-17.010	1.549
2500	9.524	70.905	63.176	19.323	-14.247	-17.125	1.497
2600	9.571	71.279	63.480	20.278	-14.250	-17.240	1.449
2700	9.615	71.641	63.775	21.237	-14.251	-17.355	1.405
2800	9.657	71.992	64.063	22.201	-14.252	-17.469	1.364
2900	9.696	72.331	64.342	23.169	-14.253	-17.582	1.325
3000	9.733	72.660	64.613	24.140	-14.254	-17.698	1.289

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 7.857 + 0.754\times10^{-3}T - 0.773\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.857\times10^{-3}T + 0.377\times10^{-6}T^2 + 0.773\times10^{2}T^{-1} - 2.635$

2000-3000 K: $Cp^\circ = 8.917 + 0.318\times10^{-3}T - 11.935\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.917\times10^{-3}T + 0.159\times10^{-6}T^2 + 11.935\times10^{2}T^{-1} - 4.441$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = -14.242 + 0.070\times10^{-3}T - 0.035\times10^{-6}T^2 + 20.550T^{-1}$

$\Delta G^\circ = -14.242 - 0.070\times10^{-3}T\ln T + 0.035\times10^{-6}T^2 + 10.275T^{-1} - 0.697\times10^{-3}T$

2000-3000 K: $\Delta H^\circ = -14.355 - 0.008\times10^{-3}T + 0.005\times10^{-6}T^2 + 248.500T^{-1}$

$\Delta G^\circ = -14.355 + 0.008\times10^{-3}T\ln T - 0.005\times10^{-6}T^2 + 124.250T^{-1} - 1.188\times10^{-3}T$

Source: Data from JANAF (53).

$SO_2(g)$

Sulfur Dioxide (ideal gas)

[Formation: $S(c,l) + O_2(g) = SO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.530	59.300	59.300	0	-70.940	-71.725	52.575
300	9.547	59.359	59.300	.018	-70.945	-71.730	52.254
368.3	10.126	61.377	59.501	.691	-71.139	-71.888	42.658
368.3	10.126	61.377	59.501	.691	-71.235	-71.888	42.658
388.36	10.296	61.918	59.612	.896	-71.293	-71.921	40.473
388.36	10.296	61.918	59.612	.896	-71.706	-71.921	40.473
400	10.395	62.224	59.684	1.016	-71.757	-71.927	39.299
432.02	10.631	63.034	59.903	1.353	-71.915	-71.935	36.390
500	11.132	64.625	60.439	2.093	-72.348	-71.902	31.428
600	11.723	66.709	61.314	3.237	-72.816	-71.766	26.140
700	12.180	68.552	62.219	4.433	-73.198	-71.560	22.342
717.824	12.243	68.859	62.380	4.651	-73.258	-71.517	21.774

Phase changes: 368.3 K, orthorhombic - monoclinic transformation of S; $\Delta H°$ = 0.096 kcal/mol.
388.36 K, melting point of S; $\Delta H°$ = 0.413 kcal/mol.
432.02 K, second order transformation of S; $\Delta H°$ = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:
$$Cp° = 11.324 + 1.592\times10^{-3}T - 2.017\times10^{5}T^{-2}$$
$$H°- H°_{298} = 11.324\times10^{-3}T + 0.796\times10^{-6}T^{2} + 2.017\times10^{2}T^{-1} - 4.124$$

2000-3000 K:
$$Cp° = 13.942 + 0.138\times10^{-3}T - 11.986\times10^{5}T^{-2}$$
$$H°- H°_{298} = 13.942\times10^{-3}T + 0.069\times10^{-6}T^{2} + 11.986\times10^{2}T^{-1} - 6.950$$

Formation equations (kcal/mol):

298.15-368.3 K:
$$\Delta Hf° = -69.905 - 4.080\times10^{-3}T + 2.010\times10^{-6}T^{2} + 0.900T^{-1}$$
$$\Delta Gf° = -69.905 + 4.080\times10^{-3}T\ln T - 2.010\times10^{-6}T^{2} + 0.450T^{-1} - 28.757\times10^{-3}T$$

368.3-388.36 K:
$$\Delta Hf° = -71.020 - 1.817\times10^{-3}T + 0.264\times10^{-6}T^{2} + 156.500T^{-1}$$
$$\Delta Gf° = -71.020 + 1.817\times10^{-3}T\ln T - 0.264\times10^{-6}T^{2} + 78.250T^{-1} - 13.574\times10^{-3}T$$

388.36-432.02 K:
$$\Delta Hf° = -87.179 + 42.923\times10^{-3}T - 43.018\times10^{-6}T^{2} + 2058.700T^{-1}$$
$$\Delta Gf° = -87.179 - 42.923\times10^{-3}T\ln T + 43.018\times10^{-6}T^{2} + 1029.350T^{-1} + 271.655\times10^{-3}T$$

432.02-717.824 K:
$$\Delta Hf° = -96.657 + 39.017\times10^{-3}T - 23.206\times10^{-6}T^{2} + 5285.200T^{-1}$$
$$\Delta Gf° = -96.657 - 39.017\times10^{-3}T\ln T + 23.206\times10^{-6}T^{2} + 2642.600T^{-1} + 269.807\times10^{-3}T$$

Sources: Enthalpy of fromation at 298 K from CODATA (36). All other data from JANAF (51).

$SO_2(g)$

Sulfur Dioxide (ideal gas)

[Reaction: $0.5S_2(g) + O_2(g) = SO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta H°$	$\Delta G°$	
298.15	9.530	59.300	59.300	0	-86.295	-81.239	59.549
300	9.547	59.359	59.300	.018	-86.297	-81.207	59.158
400	10.395	62.224	59.684	1.016	-86.408	-79.493	43.432
500	11.132	64.625	60.439	2.093	-86.476	-77.755	33.986
600	11.723	66.709	61.314	3.237	-86.511	-76.007	27.685
700	12.180	68.552	62.219	4.433	-86.523	-74.255	23.183
800	12.532	70.202	63.116	5.669	-86.521	-72.503	19.807
900	12.806	71.695	63.987	6.937	-86.507	-70.752	17.181
1000	13.022	73.056	64.827	8.229	-86.485	-69.003	15.080
1100	13.194	74.305	65.632	9.540	-86.461	-67.254	13.362
1200	13.335	75.460	66.405	10.866	-86.434	-65.511	11.931
1300	13.451	76.532	67.143	12.206	-86.404	-63.768	10.720
1400	13.549	77.532	67.849	13.556	-86.377	-62.028	9.683
1500	13.632	78.470	68.527	14.915	-86.350	-60.291	8.784
1600	13.704	79.352	69.176	16.282	-86.325	-58.554	7.998
1700	13.767	80.185	69.799	17.656	-86.303	-56.819	7.304
1800	13.822	80.973	70.398	19.035	-86.284	-55.083	6.688
1900	13.872	81.722	70.975	20.420	-86.268	-53.351	6.137
2000	13.917	82.435	71.530	21.809	-86.257	-51.620	5.641
2100	13.958	83.115	72.066	23.203	-86.249	-49.888	5.192
2200	13.995	83.765	72.583	24.601	-86.244	-48.157	4.784
2300	14.030	84.388	73.083	26.002	-86.245	-46.426	4.411
2400	14.063	84.986	73.566	27.407	-86.249	-44.695	4.070
2500	14.093	85.560	74.034	28.815	-86.256	-42.961	3.756
2600	14.122	86.114	74.489	30.225	-86.269	-41.233	3.466
2700	14.149	86.647	74.929	31.639	-86.283	-39.499	3.197
2800	14.175	87.162	75.357	33.055	-86.303	-37.763	2.948
2900	14.200	87.660	75.772	34.474	-86.325	-36.029	2.715
3000	14.224	88.142	76.177	35.895	-86.352	-34.297	2.499

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.324 + 1.592\times10^{-3}T - 2.017\times10^{5}T^{-2}$

$H°- H°_{298} = 11.324\times10^{-3}T + 0.796\times10^{-6}T^{2} + 2.017\times10^{2}T^{-1} - 4.124$

2000-3000 K: $Cp° = 13.942 + 0.138\times10^{-3}T - 11.986\times10^{5}T^{-2}$

$H°- H°_{298} = 13.942\times10^{-3}T + 0.069\times10^{-6}T^{2} + 11.986\times10^{2}T^{-1} - 6.950$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H° = -86.694 - 0.078\times10^{-3}T + 0.133\times10^{-6}T^{2} + 122.350T^{-1}$

$\Delta G° = -86.694 + 0.078\times10^{-3}T\ln T - 0.133\times10^{-6}T^{2} + 61.175T^{-1} + 17.206\times10^{-3}T$

2000-3000 K: $\Delta H° = -87.159 + 0.847\times10^{-3}T - 0.190\times10^{-6}T^{2} - 61.400T^{-1}$

$\Delta G° = -87.159 - 0.847\times10^{-3}T\ln T + 0.190\times10^{-6}T^{2} - 30.700T^{-1} + 23.843\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (36). All other data from JANAF (51).

$SO_3(g)$

Sulfur Trioxide (ideal gas)

[Formation: $S(c,l) + 1.5O_2(g) = SO_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.108	61.344	61.344	0	-94.580	-88.669	64.996
300	12.142	61.419	61.346	.022	-94.588	-88.633	64.568
368.3	13.263	64.029	61.604	.893	-94.824	-87.251	51.774
368.3	13.263	64.029	61.604	.893	-94.920	-87.251	51.774
388.36	13.593	64.742	61.748	1.163	-94.985	-86.831	48.863
388.36	13.593	64.742	61.748	1.163	-95.398	-86.831	48.863
400	13.784	65.146	61.841	1.322	-95.453	-86.573	47.301
432.02	14.200	66.223	62.126	1.770	-95.615	-85.857	43.433
500	15.082	68.367	62.831	2.768	-96.040	-84.284	36.840
600	16.075	71.209	63.996	4.328	-96.469	-81.890	29.828
700	16.824	73.746	65.210	5.975	-96.790	-79.434	24.800
717.824	16.925	74.170	65.428	6.276	-96.837	-78.991	24.049

Phase changes: 368.3 K, orthorhombic-monoclinic transformation of S; $\Delta H° = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H° = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H° = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:

$$Cp° = 16.016 + 2.098\times10^{-3}T - 4.029\times10^{5}T^{-2}$$

$$H°- H°_{298} = 16.016\times10^{-3}T + 1.049\times10^{-6}T^{2} + 4.029\times10^{2}T^{-1} - 6.220$$

2000-3000 K:

$$Cp° = 18.915 + 0.274\times10^{-3}T - 2.782\times10^{5}T^{-2}$$

$$H°- H°_{298} = 18.915\times10^{-3}T + 0.137\times10^{-6}T^{2} + 2.782\times10^{2}T^{-1} - 8.308$$

Formation equations (kcal/mol):

298.15-368.3 K:

$$\Delta Hf° = -94.466 - 3.003\times10^{-3}T + 2.012\times10^{-6}T^{2} + 179.500T^{-1}$$

$$\Delta Gf° = -94.466 + 3.003\times10^{-3}T\ln T - 2.012\times10^{-6}T^{2} + 89.750T^{-1} + 1.921\times10^{-3}T$$

368.3-388.36 K:

$$\Delta Hf° = -95.581 - 0.740\times10^{-3}T + 0.265\times10^{-6}T^{2} + 335.100T^{-1}$$

$$\Delta Gf° = -95.581 + 0.740\times10^{-3}T\ln T - 0.265\times10^{-6}T^{2} + 167.550T^{-1} + 17.104\times10^{-3}T$$

388.36-432.02 K:

$$\Delta Hf° = -111.739 + 44.000\times10^{-3}T - 43.016\times10^{-6}T^{2} + 2237.300T^{-1}$$

$$\Delta Gf° = -111.739 - 44.000\times10^{-3}T\ln T + 43.016\times10^{-6}T^{2} + 1118.650T^{-1} + 302.332\times10^{-3}T$$

432.02-717.824 K:

$$\Delta Hf° = -121.218 + 40.094\times10^{-3}T - 23.205\times10^{-6}T^{2} + 5463.800T^{-1}$$

$$\Delta Gf° = -121.218 - 40.094\times10^{-3}T\ln T + 23.205\times10^{-6}T^{2} + 2731.900T^{-1} + 300.485\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from JANAF (51).

$SO_3(g)$

Sulfur Trioxide (ideal gas)

[Reaction: $0.5S_2(g) + 1.5O_2(g) = SO_3(g)$]

T, K	cal/mol•K			kcal/mol			Log K
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔH°	ΔG°	
298.15	12.108	61.344	61.344	0	-109.935	-98.183	71.969
300	12.142	61.419	61.346	.022	-109.939	-98.110	71.472
400	13.784	65.146	61.841	1.322	-110.104	-94.139	51.434
500	15.082	68.367	62.831	2.768	-110.168	-90.137	39.399
600	16.075	71.209	63.996	4.328	-110.164	-86.131	31.373
700	16.824	73.746	65.210	5.975	-110.115	-82.129	25.641
800	17.391	76.031	66.422	7.687	-110.035	-78.137	21.346
900	17.823	78.105	67.607	9.448	-109.935	-74.156	18.007
1000	18.157	80.001	68.753	11.248	-109.819	-70.187	15.339
1100	18.419	81.745	69.857	13.077	-109.696	-66.230	13.158
1200	18.628	83.357	70.915	14.930	-109.566	-62.283	11.343
1300	18.796	84.855	71.930	16.802	-109.433	-58.348	9.809
1400	18.933	86.253	72.904	18.688	-109.301	-54.424	8.496
1500	19.046	87.563	73.838	20.587	-109.169	-50.510	7.359
1600	19.140	88.795	74.734	22.497	-109.040	-46.602	6.366
1700	19.219	89.958	75.596	24.415	-108.915	-42.704	5.490
1800	19.286	91.058	76.425	26.340	-108.794	-38.810	4.712
1900	19.344	92.103	77.223	28.272	-108.678	-34.928	4.018
2000	19.393	93.096	77.992	30.209	-108.568	-31.048	3.393
2100	19.436	94.044	78.734	32.150	-108.465	-27.176	2.828
2200	19.474	94.949	79.451	34.096	-108.368	-23.307	2.315
2300	19.507	95.815	80.143	36.045	-108.279	-19.442	1.847
2400	19.536	96.646	80.814	37.997	-108.196	-15.582	1.419
2500	19.562	97.444	81.463	39.952	-108.120	-11.725	1.025
2600	19.585	98.212	82.093	41.909	-108.051	-7.872	.662
2700	19.605	98.951	82.703	43.869	-107.987	-4.019	.325
2800	19.623	99.664	83.296	45.830	-107.932	-.166	.013
2900	19.640	100.353	83.873	47.793	-107.884	3.682	-.278
3000	19.655	101.019	84.433	49.758	-107.842	7.526	-.548

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 16.016 + 2.098X10^{-3}T - 4.029X10^{5}T^{-2}$

$H°- H°_{298} = 16.016x10^{-3}T + 1.049x10^{-6}T^2 + 4.029x10^{2}T^{-1} - 6.220$

2000-3000 K: $Cp° = 18.915 + 0.274x10^{-3}T - 2.782x10^{5}T^{-2}$

$H°- H°_{298} = 18.915x10^{-3}T + 0.137x10^{-6}T^2 + 2.782x10^{2}T^{-1} - 8.308$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H° = -111.254 + 1.000x10^{-3}T + 0.134x10^{-6}T^2 + 300.950T^{-1}$

$\Delta G° = -111.254 - 1.000x10^{-3}T\ln T - 0.134x10^{-6}T^2 + 150.475T^{-1} + 47.884x10^{-3}T$

2000-3000 K: $\Delta H° = -110.312 + 1.650x10^{-3}T - 0.227x10^{-6}T^2 - 1296.800T^{-1}$

$\Delta G° = -110.312 - 1.650x10^{-3}T\ln T + 0.227x10^{-6}T^2 - 648.400T^{-1} + 51.835x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from JANAF (51).

Sb(c,l)

Antimony

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.030	10.880	10.880	0
300	6.030	10.920	10.883	.011
400	6.200	12.680	11.123	.623
500	6.330	14.080	11.580	1.250
600	6.480	15.240	12.090	1.890
700	6.710	16.260	12.619	2.549
800	7.020	17.170	13.126	3.235
900	7.390	18.020	13.626	3.955
903.9	7.400	18.050	13.645	3.984
903.9	7.500	23.310	13.645	8.734
1000	7.500	24.060	14.606	9.454
1100	7.500	24.780	15.504	10.204
1200	7.500	25.430	16.302	10.954
1300*	7.500	26.030	17.027	11.704
1400	7.500	26.590	17.694	12.454
1500	7.500	27.110	18.307	13.204
1600	7.500	27.590	18.869	13.954
1700	7.500	28.040	19.391	14.704
1800	7.500	28.470	19.884	15.454
1860	7.500	28.720	20.169	15.904

*Data extrapolated above 1200 K.

Phase changes: 903.9 K, melting point of Sb; ΔH° = 4.750 kcal/mol.
1860 K, boiling point of Sb equilbrium mixture of Sb(g), Sb_2(g), and Sb_4(g).

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-903.9 K: $Cp^\circ = 5.088 + 2.344\times10^{-3}T + 0.216\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.088\times10^{-3}T + 1.172\times10^{-6}T^2 - 0.216\times10^{2}T^{-1} - 1.549$

903.9-1860 K: $Cp^\circ = 7.500$

$H^\circ - H^\circ_{298} = 7.500\times10^{-3}T + 1.955$

Source: Data from Hultgren (99) who extrapolated above 1200 K by assuming constant heat capacity.

Sb(g)

Antimony (ideal monatomic gas)

[Formation: Sb(c,1) = Sb(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	43.059	43.059	0	62.700	53.106	-38.927
300	4.968	43.090	43.060	.009	62.698	53.047	-38.644
400	4.968	44.519	43.254	.506	62.583	49.847	-27.235
500	4.968	45.628	43.622	1.003	62.453	46.679	-20.403
600	4.968	46.533	44.033	1.500	62.310	43.534	-15.857
700	4.968	47.299	44.448	1.996	62.147	40.420	-12.619
800	4.968	47.962	44.846	2.493	61.958	37.324	-10.196
900	4.969	48.548	45.226	2.990	61.735	34.260	-8.319
903.9	4.969	48.569	45.240	3.009	61.725	34.142	-8.255
903.9	4.969	48.569	45.240	3.009	56.975	34.142	-8.255
1000	4.970	49.071	45.584	3.487	56.733	31.722	-6.933
1100	4.973	49.545	45.923	3.984	56.480	29.239	-5.809
1200	4.979	49.978	46.243	4.482	56.228	26.770	-4.875
1300	4.989	50.377	46.546	4.980	55.976	24.325	-4.089
1400	5.004	50.747	46.833	5.479	55.725	21.905	-3.420
1500	5.027	51.093	47.106	5.981	55.477	19.503	-2.841
1600	5.056	51.418	47.365	6.485	55.231	17.106	-2.337
1700	5.094	51.726	47.612	6.993	54.989	14.723	-1.893
1800	5.140	52.018	47.849	7.504	54.750	12.364	-1.501
1860	5.172	52.188	47.987	7.814	54.610	10.960	-1.288

Phase changes: 903.9 K, melting point of Sb; $\Delta H° = 4.750$ kcal/mol.
1860 K, boiling point of Sb to equilibrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.898 + 0.094\times10^{-3}T + 0.037\times10^{5}T^{-2}$

$H°- H°_{298} = 4.898\times10^{-3}T + 0.047\times10^{-6}T^{2} - 0.037\times10^{2}T^{-1} - 1.452$

Formation equations (kcal/mol):

298.15-903.9 K: $\Delta Hf° = 62.797 - 0.190\times10^{-3}T - 1.125\times10^{-6}T^{2} + 17.900T^{-1}$

$\Delta Gf° = 62.797 + 0.190\times10^{-3}T\ln T + 1.125\times10^{-6}T^{2} + 8.950T^{-1} - 34.022\times10^{-3}T$

903.9-1860 K: $\Delta Hf° = 59.293 - 2.602\times10^{-3}T + 0.047\times10^{-6}T^{2} - 3.700T^{-1}$

$\Delta Gf° = 59.293 + 2.602\times10^{-3}T\ln T - 0.047\times10^{-6}T^{2} - 1.850T^{-1} - 45.491\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from Hilsenrath (94).

Sb(g)

Antimony (ideal monatomic gas)

[Reaction: $0.5Sb_2(g) = Sb(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	4.968	43.059	43.059	0	34.550	30.791	-22.570
300	4.968	43.090	43.060	.009	34.551	30.767	-22.414
400	4.968	44.519	43.254	.506	34.610	29.496	-16.116
500	4.968	45.628	43.622	1.003	34.667	28.213	-12.332
600	4.968	46.533	44.033	1.500	34.720	26.917	-9.804
700	4.968	47.299	44.448	1.996	34.772	25.611	-7.996
800	4.968	47.962	44.846	2.493	34.824	24.299	-6.638
900	4.969	48.548	45.226	2.990	34.876	22.981	-5.580
1000	4.970	49.071	45.584	3.487	34.927	21.656	-4.733
1100	4.973	49.545	45.923	3.984	34.978	20.327	-4.039
1200	4.979	49.978	46.243	4.482	35.030	18.993	-3.459
1300	4.989	50.377	46.546	4.980	35.082	17.654	-2.968
1400	5.004	50.747	46.833	5.479	35.134	16.311	-2.546
1500	5.027	51.093	47.106	5.981	35.189	14.965	-2.180
1600	5.056	51.418	47.365	6.485	35.247	13.615	-1.860
1700	5.094	51.726	47.612	6.993	35.308	12.261	-1.576
1800	5.140	52.018	47.849	7.504	35.372	10.903	-1.324
1900	5.194	52.298	48.076	8.021	35.443	9.542	-1.098
2000	5.256	52.566	48.295	8.543	35.518	8.176	-.893

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 4.898 + 0.094\times10^{-3}T + 0.037\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.898\times10^{-3}T + 0.047\times10^{-6}T^2 - 0.037\times10^{2}T^{-1} - 1.452$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = 34.463 + 0.431\times10^{-3}T + 0.047\times10^{-6}T^2 - 13.700T^{-1}$

$\Delta G^\circ = 34.463 - 0.431\times10^{-3}T\ln T - 0.047\times10^{-6}T^2 - 6.850T^{-1} - 9.768\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from Hilsenrath (94).

$Sb_2(g)$

Antimony (ideal diatomic gas)

[Formation: $2Sb(c,l) = Sb_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.690	60.900	60.900	0	56.300	44.630	-32.715
300	8.692	60.954	60.901	.016	56.294	44.560	-32.461
400	8.794	63.470	61.240	.892	55.946	40.702	-22.238
500	8.848	65.440	61.896	1.772	55.572	36.932	-16.143
600	8.876	67.056	62.623	2.660	55.180	33.234	-12.105
700	8.892	68.424	63.355	3.548	54.750	29.617	-9.247
800	8.904	69.612	64.064	4.438	54.268	26.050	-7.117
900	8.912	70.662	64.742	5.328	53.718	22.558	-5.478
903.9	8.912	70.701	64.768	5.363	53.695	22.424	-5.422
903.9	8.912	70.701	64.768	5.363	44.195	22.424	-5.422
1000	8.916	71.600	65.380	6.220	43.612	20.132	-4.400
1100	8.922	72.452	65.987	7.112	43.004	17.823	-3.541
1200	8.926	73.228	66.558	8.004	42.396	15.554	-2.833
1300	8.928	73.942	67.099	8.896	41.788	13.341	-2.243
1400	8.928	74.604	67.611	9.790	41.182	11.188	-1.747
1500	8.930	75.220	68.097	10.684	40.576	9.076	-1.322
1600	8.932	75.796	68.561	11.576	39.968	6.982	-.954
1700	8.932	76.338	69.003	12.470	39.362	4.923	-.633
1800	8.934	76.848	69.424	13.364	38.756	2.922	-.355
1860	8.935	77.142	69.670	13.899	38.391	1.745	-.205

Phase changes: 903.9 K, melting point of Sb; $\Delta H°$ = 4.750 kcal/mol.
1860 K, melting point of Sb to equilibrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.933 - 0.200\times10^{5}T^{-2}$

$H°- H°_{298} = 8.933\times10^{-3}T + 0.200\times10^{2}T^{-1} - 2.730$

Formation equations (kcal/mol):

298.15-903.9 K: $\Delta Hf° = 56.667 - 1.243\times10^{-3}T - 2.344\times10^{-6}T^{2} + 63.200T^{-1}$

$\Delta Gf° = 56.667 + 1.243\times10^{-3}T\ln T + 2.344\times10^{-6}T^{2} + 31.600T^{-1} - 48.507\times10^{-3}T$

903.9-1860 K: $\Delta Hf° = 49.660 - 6.067\times10^{-3}T + 20.000T^{-1}$

$\Delta Gf° = 49.660 + 6.067\times10^{-3}T\ln T + 10.000T^{-1} - 71.446\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from Hultgren (99).

$Sb_2(g)$

Antimony (ideal diatomic gas)

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	8.690	60.900	60.900	0
300	8.692	60.954	60.901	.016
400	8.794	63.470	61.240	.892
500	8.848	65.440	61.896	1.772
600	8.876	67.056	62.623	2.660
700	8.892	68.424	63.355	3.548
800	8.904	69.612	64.064	4.438
900	8.912	70.662	64.742	5.328
1000	8.916	71.600	65.380	6.220
1100	8.922	72.452	65.987	7.112
1200	8.926	73.228	66.558	8.004
1300	8.928	73.942	67.099	8.896
1400	8.928	74.604	67.611	9.790
1500	8.930	75.220	68.097	10.684
1600	8.932	75.796	68.561	11.576
1700	8.932	76.338	69.003	12.470
1800	8.934	76.848	69.424	13.364
1900	8.936	77.332	69.829	14.256
2000	8.936	77.790	70.215	15.150

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15–2000 K: $Cp^\circ = 8.933 - 0.200\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.933\times10^{-3}T + 0.200\times10^{2}T^{-1} - 2.730$

Source: Data from Hultgren (99).

$Sb_4(g)$

Antimony (ideal tetratomic gas)

[Formation: $4Sb(c,l) = Sb_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.352	83.652	83.652	0	49.000	37.035	-27.147
300	19.356	83.772	83.652	.036	48.992	36.964	-26.928
400	19.552	89.368	84.408	1.984	48.492	33.033	-18.048
500	19.656	93.748	85.860	3.944	47.944	29.230	-12.776
600	19.716	97.336	87.483	5.912	47.352	25.526	-9.298
700	19.760	100.380	89.111	7.888	46.692	21.954	-6.854
800	19.788	103.020	90.690	9.864	45.924	18.452	-5.041
900	19.808	105.348	92.188	11.844	45.024	15.083	-3.663
903.9	19.808	105.434	92.245	11.921	44.985	14.954	-3.616
903.9	19.808	105.434	92.245	11.921	25.985	14.954	-3.616
1000	19.816	107.436	93.612	13.824	25.008	13.812	-3.019
1100	19.828	109.328	94.957	15.808	23.992	12.763	-2.536
1200	19.832	111.052	96.225	17.792	22.976	11.778	-2.145
1300	19.836	112.640	97.431	19.772	21.956	10.880	-1.829
1400	19.840	114.108	98.568	21.756	20.940	10.093	-1.576
1500	19.844	115.480	99.653	23.740	19.924	9.364	-1.364
1600	19.848	116.760	100.680	25.728	18.912	8.672	-1.185
1700	19.848	117.964	101.663	27.712	17.896	8.029	-1.032
1800	19.852	119.096	102.598	29.696	16.880	7.491	-.910
1860	19.852	119.750	103.144	30.886	16.270	7.212	-.847

Phase changes: 903.9 K, melting point of Sb; ΔH° = 4.750 kcal/mol.
1860 K, boiling point of Sb to equilibrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.816 + 0.034\times10^{-3}T - 0.422\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.816\times10^{-3}T + 0.017\times10^{-6}T^2 + 0.422\times10^{2}T^{-1} - 6.051$

Formation equations (kcal/mol):

298.15-903.9 K: $\Delta Hf^\circ = 49.144 - 0.536\times10^{-3}T - 4.671\times10^{-6}T^2 + 128.600T^{-1}$

$\Delta Gf^\circ = 49.144 + 0.536\times10^{-3}T\ln T + 4.671\times10^{-6}T^2 + 64.300T^{-1} - 45.784\times10^{-3}T$

903.9-1860 K: $\Delta Hf^\circ = 35.130 - 10.184\times10^{-3}T + 0.017\times10^{-6}T^2 + 42.200T^{-1}$

$\Delta Gf^\circ = 35.130 + 10.184\times10^{-3}T\ln T - 0.017\times10^{-6}T^2 + 21.100T^{-1} - 91.661\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from Hultgren (99).

$Sb_4(g)$

Antimony (ideal tetratomic gas)

[Reaction: $2Sb_2(g) = Sb_4(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	19.352	83.652	83.652	0	-63.600	-52.226	38.282
300	19.356	83.772	83.652	.036	-63.596	-52.155	37.995
400	19.552	89.368	84.408	1.984	-63.400	-48.371	26.428
500	19.656	93.748	85.860	3.944	-63.200	-44.634	19.509
600	19.716	97.336	87.483	5.912	-63.008	-40.942	14.913
700	19.760	100.380	89.111	7.888	-62.808	-37.280	11.639
800	19.788	103.020	90.690	9.864	-62.612	-33.649	9.192
900	19.808	105.348	92.188	11.844	-62.412	-30.034	7.293
1000	19.816	107.436	93.612	13.824	-62.216	-26.452	5.781
1100	19.828	109.328	94.957	15.808	-62.016	-22.882	4.546
1200	19.832	111.052	96.225	17.792	-61.816	-19.331	3.521
1300	19.836	112.640	97.431	19.772	-61.620	-15.803	2.657
1400	19.840	114.108	98.568	21.756	-61.424	-12.284	1.918
1500	19.844	115.480	99.653	23.740	-61.228	-8.788	1.280
1600	19.848	116.760	100.680	25.728	-61.024	-5.293	.723
1700	19.848	117.964	101.663	27.712	-60.828	-1.818	.234
1800	19.852	119.096	102.598	29.696	-60.632	1.648	-.200
1900	19.852	120.172	103.498	31.680	-60.432	5.103	-.587
2000	19.852	121.188	104.356	33.664	-60.236	8.548	-.934

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.816 + 0.034\times10^{-3}T - 0.422\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.816\times10^{-3}T + 0.017\times10^{-6}T^2 + 0.422\times10^{2}T^{-1} - 6.051$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = -64.190 + 1.950\times10^{-3}T + 0.017\times10^{-6}T^2 + 2.200T^{-1}$

$\Delta G^\circ = -64.190 - 1.950\times10^{-3}T\ln T - 0.017\times10^{-6}T^2 + 1.100T^{-1} + 51.231\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from Hultgren (99).

Sb_2O_3(orthorhombic)

Diantimony Trioxide, Antimony Sesquioxide

[Formation: $2Sb(c,1) + 1.5O_2(g) = Sb_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	24.230	29.400	29.400	0	-169.400	-149.762	109.777
300*	24.278	29.550	29.400	.045	-169.396	-149.637	109.009
400	26.036	36.809	30.379	2.572	-169.158	-143.084	78.177
500	26.955	42.726	32.274	5.226	-168.855	-136.597	59.706
600	27.550	47.696	34.441	7.953	-168.540	-130.183	47.418
700	27.991	51.978	36.648	10.731	-168.247	-123.807	38.654
800	28.350	55.739	38.804	13.548	-167.999	-117.487	32.095
900	28.662	59.097	40.876	16.399	-167.809	-111.180	26.998
903.9	28.673	59.221	40.955	16.511	-167.804	-110.934	26.822
903.9	28.673	59.221	40.955	16.511	-177.304	-110.934	26.822
928	28.743	59.976	41.442	17.200	-177.274	-109.163	25.708

*Data above 298 K estimated.

Phase changes: 879 K, cubic - orthorhombic transition of Sb_2O_3: $\Delta H^\circ = 1 \pm 0.5$ kcal/mol. Orthorhombic form metastable below 879 K. Insufficient data to tabulate cubic form.
903.9 K, melting point of Sb; $\Delta H^\circ = 4.750$ kcal/mol.
928 K, melting point of Sb_2O_3. Insufficient data for enthalpy of fusion.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-928 K: $Cp^\circ = 27.250 + 1.988\times10^{-3}T - 3.211\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 27.250\times10^{-3}T + 0.994\times10^{-6}T^2 + 3.211\times10^{2}T^{-1} - 9.290$

Formation equations (kcal/mol):

298.15-903.9 K: $\Delta Hf^\circ = -172.065 + 6.229\times10^{-3}T - 2.105\times10^{-6}T^2 + 296.500T^{-1}$

$\Delta Gf^\circ = -172.065 - 6.229\times10^{-3}T\ln T + 2.105\times10^{-6}T^2 + 148.250T^{-1} + 108.000\times10^{-3}T$

903.9-928 K: $\Delta Hf^\circ = -179.071 + 1.405\times10^{-3}T + 0.239\times10^{-6}T^2 + 253.300T^{-1}$

$\Delta Gf^\circ = -179.071 - 1.405\times10^{-3}T\ln T - 0.239\times10^{-6}T^2 + 126.650T^{-1} + 85.061\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities and entropy at 298 K from Anderson (2). High-temperature data estimated.

$Sb_2O_4(c)$

Diantimony Tetroxide

[Formation: $2Sb(c,l) + 2O_2(g) = Sb_2O_4(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	27.380	30.350	30.350	0	-216.900	-190.239	139.447
300*	27.445	30.520	30.350	0.051	-216.897	-190.072	138.465
400	29.604	38.761	31.459	2.921	-216.671	-181.159	98.980
500	30.552	45.480	33.614	5.933	-216.375	-172.314	75.317
600	31.123	51.104	36.072	9.019	-216.079	-163.537	59.568
700	31.562	55.935	38.572	12.154	-215.818	-154.794	48.328
800	31.956	60.176	41.014	15.330	-215.610	-146.103	39.913
900	32.338	63.962	43.356	18.545	-215.463	-137.419	33.369
903.9	32.353	64.102	43.446	18.671	-215.459	-137.080	33.144
903.9	32.353	64.102	43.446	18.671	-224.959	-137.080	33.144
1000	32.722	67.389	45.591	21.798	-224.862	-127.751	27.920
1100	33.111	70.526	47.718	25.089	-224.749	-118.034	23.451
1200	33.510	73.424	49.741	28.420	-224.614	-108.344	19.732

*Data above 298 K estimated.

Phase change: 903.9 K, melting point of Sb; ΔH° = 4.750 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp^\circ = 31.403 + 1.580\times10^{-3}T - 3.995\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 31.403\times10^{-3}T + 0.790\times10^{-6}T^2 + 3.995\times10^{2}T^{-1} - 10.773$

Formation equations (kcal/mol):

298.15-903.9 K: $\Delta Hf^\circ = -219.872 + 6.767\times10^{-3}T - 2.560\times10^{-6}T^2 + 352.300T^{-1}$

$\Delta Gf^\circ = -219.872 - 6.767\times10^{-3}T\ln T + 2.560\times10^{-6}T^2 + 176.150T^{-1} + 135.198\times10^{-3}T$

903.9-1200 K: $\Delta Hf^\circ = -226.879 + 1.943\times10^{-3}T - 0.216\times10^{-6}T^2 + 309.100T^{-1}$

$\Delta Gf^\circ = -226.879 - 1.943\times10^{-3}T\ln T + 0.216\times10^{-6}T^2 + 154.550T^{-1} + 112.259\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities and entropy at 298 K from Anderson (2). High-temperature data estimated.

$Sb_2O_5(c)$

Diantimony Pentoxide

[Formation: $2Sb(c) + 2.5O_2(g) = Sb_2O_5(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	28.104	29.860	29.860	0	-232.300	-198.188	145.274
300*	28.175	30.034	29.861	.052	-232.303	-197.974	144.222
400	30.350	38.495	31.000	2.998	-232.355	-186.519	101.908
500	31.283	45.377	33.209	6.084	-232.351	-175.058	76.517
600	31.942	51.141	35.729	9.247	-232.356	-163.607	59.593
700	32.497	56.108	38.295	12.469	-232.397	-152.140	47.500

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 33.778 - 0.892\times10^{-3}T - 4.807\times10^{5}T^{-2}$

$H°- H°_{298} = 33.778\times10^{-3}T - 0.446\times10^{-6}T^{2} + 4.807\times10^{2}T^{-1} - 11.644$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf° = -234.966 + 5.527\times10^{-3}T - 4.048\times10^{-6}T^{2} + 410.900T^{-1}$

$\Delta Gf° = -234.966 - 5.527\times10^{-3}T\ln T + 4.048\times10^{-6}T^{2} + 205.450T^{-1} + 151.328\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities and entropy at 298 K from Anderson (2). High-temperature data estimated.

$Sb_4O_6(g)$

Tetrantimony Hexoxide (ideal gas)

[Formation: $4Sb(c,l) + 3O_2(g) = Sb_4O_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	43.680	106.140	106.140	0	-290.520	-265.358	194.510
300	43.780	106.410	106.140	.081	-290.522	-265.197	193.193
400	48.060	119.660	107.923	4.695	-290.486	-256.754	140.282
500	50.460	130.670	111.406	9.632	-290.250	-248.343	108.549
600	51.910	140.000	115.405	14.757	-289.950	-239.999	87.419
700	52.830	148.080	119.513	19.997	-289.680	-231.686	72.335
800	53.460	155.180	123.537	25.314	-289.501	-223.437	61.039
900	53.900	161.500	127.408	30.683	-289.454	-215.171	52.250
903.9	53.912	161.733	127.555	30.893	-289.456	-214.847	51.946
903.9	53.912	161.733	127.555	30.893	-308.456	-214.847	51.946
1000	54.220	167.200	131.111	36.089	-308.525	-204.915	44.784

Phase change: 903.9 K, melting point of Sb; $\Delta H° = 4.750$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 52.016 + 3.372\times10^{-3}T - 8.304\times10^{5}T^{-2}$

$H°- H°_{298} = 52.016\times10^{-3}T + 1.686\times10^{-6}T^2 + 8.304\times10^{2}T^{-1} - 18.444$

Formation equations (kcal/mol):

298.15-903.9 K: $\Delta Hf° = -295.713 + 9.974\times10^{-3}T - 4.511\times10^{-6}T^2 + 781.200T^{-1}$

$\Delta Gf° = -295.713 - 9.974\times10^{-3}T\ln T + 4.511\times10^{-6}T^2 + 390.600T^{-1} + 152.901\times10^{-3}T$

903.9-1000 K: $\Delta Hf° = -309.727 + 0.326\times10^{-3}T + 0.177\times10^{-6}T^2 + 694.800T^{-1}$

$\Delta Gf° = -309.727 - 0.326\times10^{-3}T\ln T - 0.177\times10^{-6}T^2 + 347.400T^{-1} + 107.024\times10^{-3}T$

Source: Data from Behrens (14).

Sc(c,l)

Scandium

T, K	cal/mol•K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.100	8.280	8.280	0
300	6.100	8.320	8.283	.011
400	6.290	10.100	8.520	.632
500	6.410	11.520	8.986	1.267
600	6.570	12.700	9.507	1.916
700	6.750	13.730	10.041	2.582
800	6.960	14.650	10.566	3.267
900	7.200	15.470	11.053	3.975
1000	7.460	16.240	11.532	4.708
1100	7.750	16.970	11.999	5.468
1200	8.060	17.680	12.465	6.258
1300	8.390	18.320	12.874	7.080
1400	8.750	18.950	13.280	7.938
1500	9.140	19.570	13.682	8.832
1600	9.550	20.170	14.066	9.766
1608	9.580	20.220	14.101	9.842
1608	10.570	20.820	14.101	10.800
1700	10.570	21.400	14.475	11.772
1800	10.570	22.000	14.873	12.829
1812	10.570	22.070	14.920	12.956
1812*	10.570	23.930	14.920	16.325
1900	10.570	24.430	15.348	17.255
2000	10.570	24.970	15.814	18.312
2100	10.570	25.490	16.267	19.369
2200	10.570	25.980	16.695	20.426
2300	10.570	26.450	17.110	21.483
2400	10.570	26.900	17.508	22.540
2500	10.570	27.330	17.891	23.597
2600	10.570	27.750	18.268	24.654
2700	10.570	28.150	18.627	25.711
2800	10.570	28.530	18.970	26.768
2900	10.570	28.900	19.305	27.825
3000	10.570	29.260	19.633	28.882

*Data for Sc(l) estimated.

Phase changes: 1608 K, α - β transition point of Sc; ΔH° = 0.958 kcal/mol.
1812 K, melting point of Sc; ΔH° = 3.369 kcal/mol.
3104 K, boiling point of Sc; ΔH° = 75.1 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1608 K: $Cp^\circ = 4.884 + 2.678\times10^{-3}T + 0.371\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.884\times10^{-3}T + 1.339\times10^{-6}T^2 - 0.371\times10^{2}T^{-1} - 1.451$

1608-1812 K: $Cp^\circ = 10.570$

$H^\circ - H^\circ_{298} = 10.570\times10^{-3}T - 6.197$

1812-3000 K: $Cp^\circ = 10.570$

$H^\circ - H^\circ_{298} = 10.570\times10^{-3}T - 2.828$

Source: Data from Hultgren (99) who estimated data for Sc(l).

Sc(g)

Scandium (ideal monatomic gas)

[Formation: Sc(c,1) = Sc(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.283	41.749	41.749	0	90.300	80.321	-58.876
300	5.279	41.781	41.749	.010	90.299	80.261	-58.469
400	5.148	43.279	41.954	.530	90.198	76.926	-42.030
500	5.084	44.421	42.339	1.041	90.074	73.624	-32.180
600	5.049	45.344	42.764	1.548	89.932	70.346	-25.623
700	5.027	46.121	43.190	2.052	89.770	67.096	-20.948
800	5.013	46.791	43.598	2.554	89.587	63.874	-17.449
900	5.004	47.381	43.987	3.055	89.380	60.660	-14.730
1000	4.997	47.908	44.353	3.555	89.147	57.479	-12.562
1100	4.992	48.384	44.699	4.054	88.886	54.331	-10.794
1200	4.989	48.818	45.024	4.553	88.595	51.229	-9.330
1300	4.988	49.217	45.331	5.052	88.272	48.106	-8.087
1400	4.989	49.587	45.622	5.551	87.913	45.021	-7.028
1500	4.993	49.931	45.898	6.050	87.518	41.977	-6.116
1600	5.001	50.254	46.161	6.549	87.083	38.949	-5.320
1608	5.002	50.279	46.181	6.589	87.047	38.716	-5.262
1608	5.002	50.279	46.181	6.589	86.089	38.716	-5.262
1700	5.014	50.557	46.410	7.050	85.578	36.011	-4.629
1800	5.034	50.844	46.648	7.553	85.024	33.105	-4.019
1812	5.037	50.877	46.676	7.613	84.957	32.758	-3.951
1812	5.037	50.877	46.676	7.613	81.588	32.758	-3.951
1900	5.062	51.117	46.876	8.057	81.102	30.397	-3.496
2000	5.099	51.378	47.095	8.565	80.553	27.737	-3.031
2100	5.148	51.628	47.306	9.077	80.008	25.118	-2.614
2200	5.208	51.869	47.508	9.595	79.469	22.513	-2.236
2300	5.282	52.102	47.702	10.119	78.936	19.936	-1.894
2400	5.369	52.328	47.890	10.652	78.412	17.385	-1.583
2500	5.471	52.549	48.071	11.194	77.897	14.850	-1.298

Phase changes: 1608 K, α - β transition point of Sc; $\Delta H°$ = 0.958 kcal/mol.
1812 K, melting point of Sc; $\Delta H°$ = 3.369 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 4.877 + 0.100\times10^{-3}T + 0.335\times10^{5}T^{-2}$

$H°- H°_{298} = 4.877\times10^{-3}T + 0.050\times10^{-6}T^{2} - 0.335\times10^{2}T^{-1} - 1.346$

Formation equations (kcal/mol):

298.15-1608 K: $\Delta Hf° = 90.405 - 0.007\times10^{-3}T - 1.289\times10^{-6}T^{2} + 3.600T^{-1}$

$\Delta Gf° = 90.405 + 0.007\times10^{-3}T\ln T + 1.289\times10^{-6}T^{2} + 1.800T^{-1} - 34.264\times10^{-3}T$

1608-1812 K: $\Delta Hf° = 95.151 - 5.693\times10^{-3}T + 0.050\times10^{-6}T^{2} - 33.500T^{-1}$

$\Delta Gf° = 95.151 + 5.693\times10^{-3}T\ln T - 0.050\times10^{-6}T^{2} - 16.750T^{-1} - 77.034\times10^{-3}T$

1812-2500 K: $\Delta Hf° = 91.782 - 5.693\times10^{-3}T + 0.050\times10^{-6}T^{2} - 33.500T^{-1}$

$\Delta Gf° = 91.782 + 5.693\times10^{-3}T\ln T - 0.050\times10^{-6}T^{2} - 16.750T^{-1} - 75.174\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (238). All other data from Hilsenrath (94).

$Sc_2O_3(c,1)$

Discandium Trioxide, Scandium Sesquioxide

[Formation: $2Sc(c,1) + 1.5O_2(g) = Sc_2O_3(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	22.520	18.400	18.400	0	-456.220	-434.852	318.751
300	22.588	18.540	18.400	.042	-456.220	-434.717	316.687
400	25.182	25.433	19.323	2.444	-456.125	-427.564	233.607
500	26.749	31.231	21.139	5.046	-455.889	-420.444	183.773
600	27.880	36.213	23.246	7.780	-455.586	-413.386	150.574
700	28.744	40.579	25.418	10.613	-455.251	-406.374	126.874
800	29.416	44.463	27.561	13.522	-454.909	-399.408	109.112
900	29.941	47.959	29.636	16.491	-454.578	-392.514	95.314
1000	30.352	51.136	31.630	19.506	-454.269	-385.640	84.280
1100	30.677	54.044	33.537	22.558	-453.995	-378.776	75.255
1200	30.940	56.725	35.358	25.640	-453.766	-371.893	67.730
1300	31.161	59.210	37.098	28.745	-453.589	-365.124	61.382
1400	31.359	61.527	38.762	31.871	-453.474	-358.341	55.939
1500	31.549	63.697	40.352	35.017	-453.422	-351.538	51.218
1600	31.745	65.739	41.876	38.181	-453.441	-344.754	47.091
1608	31.762	65.897	41.995	38.435	-453.445	-344.196	46.781
1608	31.762	65.897	41.995	38.435	-455.361	-344.196	46.781
1700	31.957	67.670	43.337	41.366	-455.591	-337.847	43.433
1800	32.193	69.503	44.740	44.573	-455.830	-330.928	40.180
1812	32.225	69.717	44.905	44.960	-455.858	-330.095	39.813
1812	32.225	69.717	44.905	44.960	-462.596	-330.095	39.813
1900	32.459	71.251	46.090	47.806	-462.790	-323.660	37.229
2000	32.759	72.923	47.390	51.066	-462.992	-316.340	34.568
2100	33.092	74.530	48.645	54.358	-463.172	-308.986	32.156
2200	33.459	76.077	49.856	57.686	-463.323	-301.646	29.965
2300	33.854	77.573	51.029	61.051	-463.446	-294.295	27.964
2400	34.272	79.023	52.166	64.457	-463.536	-286.939	26.129
2500	34.702	80.431	53.269	67.906	-463.590	-279.587	24.441
2600	35.136	81.800	54.339	71.398	-463.608	-272.197	22.880
2700	35.557	83.134	55.381	74.933	-463.591	-264.831	21.436
2762	35.805	83.946	56.013	77.150	-463.559	-260.288	20.596
2762	48.000	96.129	56.013	110.800	-429.909	-260.288	20.596
2800	48.000	96.785	56.562	112.624	-429.426	-257.958	20.134
2900	48.000	98.469	57.978	117.424	-428.159	-251.860	18.980
3000	48.000	100.097	59.356	122.224	-426.899	-245.797	17.906

Phase changes: 1608 K, α - β transition point of Sc; ΔH° = 0.958 kcal/mol.
1812 K, melting point of Sc; ΔH° = 3.369 kcal/mol.
2762 K, melting point of Sc_2O_3: ΔH° = 33.650 kcal/mol.

Sc_2O_3(c,l) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2762 K: $Cp^\circ = 27.709 + 2.780\times10^{-3}T - 5.351\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 27.709\times10^{-3}T + 1.390\times10^{-6}T^2 + 5.351\times10^{2}T^{-1} - 10.180$

2762-3000 K: $Cp^\circ = 48.000$

$H^\circ - H^\circ_{298} = 48.000\times10^{-3}T - 21.776$

Formation equations (kcal/mol):

298.15-1608 K: $\Delta Hf^\circ = -459.970 + 7.096\times10^{-3}T - 2.043\times10^{-6}T^2 + 541.500T^{-1}$

$\Delta Gf^\circ = -459.970 - 7.096\times10^{-3}T\ln T + 2.043\times10^{-6}T^2 + 270.750T^{-1} + 121.021\times10^{-3}T$

1608-1812 K: $\Delta Hf^\circ = -450.478 - 4.276\times10^{-3}T + 0.636\times10^{-6}T^2 + 467.300T^{-1}$

$\Delta Gf^\circ = -450.478 + 4.276\times10^{-3}T\ln T - 0.636\times10^{-6}T^2 + 233.650T^{-1} + 35.482\times10^{-3}T$

1812-2000 K: $\Delta Hf^\circ = -457.216 - 4.276\times10^{-3}T + 0.636\times10^{-6}\ \rightarrow^2 + 467\ T^{-1}$

$\Delta Gf^\circ = -457.216 + 4.276\times10^{-3}T\ln T - 0.636\times10^{-6}T^2 + 233.650T^{-1} + 39.201\times10^{-3}T$

2000-2762 K: $\Delta Hf^\circ = -455.212 - 5.941\times10^{-3}T + 1.076\times10^{-6}T^2 - 409.900T^{-1}$

$\Delta Gf^\circ = -455.212 + 5.941\times10^{-3}T\ln T - 1.076\times10^{-6}T^2 - 204.950T^{-1} + 26.535\times10^{-3}T$

2762-3000 K: $\Delta Hf^\circ = -466.808 + 14.350\times10^{-3}T - 0.314\times10^{-6}T^2 - 945.000T^{-1}$

$\Delta Gf^\circ = -466.808 - 14.350\times10^{-3}T\ln T + 0.314\times10^{-6}T^2 - 472.500T^{-1} + 187.709\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (238). Low-temperature heat capacities and entropy at 298 K from Weller (242). High-temperature data based on Pankratz (175) and Shpil'rain (201).

Se(c,1)

Selenium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.987	10.144	10.144	0
300	5.989	10.181	10.144	.011
400	6.319	11.950	10.382	.627
494.3	6.525	13.308	10.812	1.234
494.3	8.592	16.286	10.812	2.706
500	8.568	16.384	10.874	2.755
600	8.238	17.916	11.924	3.595
700	8.016	19.169	12.873	4.407
800	7.956	20.232	13.728	5.203
900	8.109	21.176	14.504	6.005
958	8.312	21.690	14.926	6.480

Phase changes: 494.3 K, melting point of Se; ΔH° = 1.472 kcal/mol.
958 K, boiling point of Se to equilibrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-494.3 K: $Cp^\circ = 5.462 + 2.368\times10^{-3}T - 0.161\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.462\times10^{-3}T + 1.184\times10^{-6}T^2 + 0.161\times10^{2}T^{-1} - 1.788$

494.3-958 K: $Cp^\circ = 6.434 + 1.256\times10^{-3}T + 3.756\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.434\times10^{-3}T + 0.628\times10^{-6}T^2 - 3.756\times10^{2}T^{-1} + 0.132$

Sources: Entropy at 298 K from Wagman (236). All other data from Gronvold (84).

Se(g)

Selenium (ideal monatomic gas)

[Reaction: $0.5Se_2(g) = Se(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	4.990	42.210	42.210	0	39.600	35.691	-26.162
300	4.990	42.240	42.210	.009	39.600	35.667	-25.983
400	5.140	43.700	42.408	.517	39.611	34.354	-18.770
500	5.220	44.860	42.790	1.035	39.625	33.037	-14.440
600	5.280	45.820	43.220	1.560	39.644	31.715	-11.552
700	5.340	46.630	43.641	2.092	39.671	30.399	-9.491
800	5.380	47.350	44.065	2.628	39.703	29.071	-7.942
900	5.430	47.990	44.470	3.168	39.741	27.735	-6.735
1000	5.470	48.560	44.847	3.713	39.787	26.402	-5.770
1100	5.510	49.080	45.205	4.262	39.839	25.066	-4.980
1200	5.550	49.560	45.548	4.814	39.896	23.721	-4.320
1300	5.580	50.010	45.878	5.371	39.962	22.366	-3.760
1400	5.620	50.430	46.194	5.931	40.034	21.000	-3.278
1500	5.660	50.810	46.479	6.496	40.113	19.653	-2.863
1600	5.700	51.180	46.766	7.063	40.198	18.278	-2.497
1700	5.730	51.530	47.039	7.635	40.290	16.907	-2.173
1800	5.770	51.860	47.299	8.210	40.389	15.521	-1.885
1900	5.810	52.170	47.544	8.789	40.494	14.141	-1.627
2000	5.840	52.470	47.784	9.372	40.607	12.747	-1.393

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 5.132 + 0.358\times10^{-3}T - 0.221\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.132\times10^{-3}T + 0.179\times10^{-6}T^2 + 0.221\times10^{2}T^{-1} - 1.620$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = 39.656 - 0.200\times10^{-3}T + 0.338\times10^{-6}T^2 - 7.850T^{-1}$

$\Delta G^\circ = 39.656 + 0.200\times10^{-3}T\ln T - 0.338\times10^{-6}T^2 - 3.925T^{-1} - 14.292\times10^{-3}T$

Source: Data from Mills (158).

$Se_2(g)$

Selenium (ideal diatomic gas)

[Formation: $2Se(c,1) = Se_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.800	58.200	58.200	0	33.300	21.997	-16.124
300	9.810	58.260	58.200	.018	33.296	21.927	-15.973
400	10.030	61.120	58.587	1.013	33.059	18.171	-9.928
494.3	10.096	63.254	59.282	1.963	32.795	14.685	-6.493
494.3	10.096	63.254	59.282	1.963	29.851	14.685	-6.493
500	10.100	63.370	59.328	2.021	29.811	14.510	-6.342
600	10.110	65.210	60.157	3.032	29.142	11.515	-4.194
700	10.090	66.770	60.996	4.042	28.528	8.626	-2.693
800	10.060	68.120	61.808	5.050	27.944	5.819	-1.590
900	10.010	69.300	62.573	6.054	27.344	3.091	-.751
958	9.987	69.922	62.997	6.634	26.974	1.547	-.353

Phase changes: 494.3 K, melting point of Se; $\Delta H° = 1.472$ kcal/mol.
958 K, boiling point of Se to equilbrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.664 - 0.638\times10^{-3}T - 0.599\times10^{5}T^{-2}$

$H°- H°_{298} = 10.664\times10^{-3}T - 0.319\times10^{-6}T^{2} + 0.599\times10^{2}T^{-1} - 3.352$

Formation equations (kcal/mol):

298.15-494.3 K: $\Delta Hf° = 33.523 - 0.260\times10^{-3}T - 2.687\times10^{-6}T^{2} + 27.700T^{-1}$

$\Delta Gf° = 33.523 + 0.260\times10^{-3}T\ln T + 2.687\times10^{-6}T^{2} + 13.850T^{-1} - 41.100\times10^{-3}T$

494.3-958 K: $\Delta Hf° = 29.684 - 2.204\times10^{-3}T - 1.575\times10^{-6}T^{2} + 811.100T^{-1}$

$\Delta Gf° = 29.684 + 2.204\times10^{-3}T\ln T + 1.575\times10^{-6}T^{2} + 405.550T^{-1} - 46.444\times10^{-3}T$

Source: Data from Mills (158).

$Se_2(g)$

Selenium (ideal diatomic gas)

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	9.800	58.200	58.200	0
300	9.810	58.260	58.200	.018
400	10.030	61.120	58.587	1.013
500	10.100	63.370	59.328	2.021
600	10.110	65.210	60.157	3.032
700	10.090	66.770	60.996	4.042
800	10.060	68.120	61.808	5.050
900	10.010	69.300	62.573	6.054
1000	9.970	70.350	63.297	7.053
1100	9.910	71.300	63.985	8.047
1200	9.860	72.160	64.631	9.035
1300	9.800	72.950	65.244	10.018
1400	9.740	73.670	65.816	10.995
1500	9.680	74.340	66.363	11.966
1600	9.620	74.960	66.878	12.931
1700	9.560	75.550	67.379	13.890
1800	9.500	76.090	67.844	14.843
1900	9.440	76.600	68.289	15.790
2000	9.380	77.080	68.715	16.730

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 10.664 - 0.638\times10^{-3}T - 0.599\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.664\times10^{-3}T - 0.319\times10^{-6}T^{2} + 0.599\times10^{2}T^{-1} - 3.352$

Source: Data from Mills (158).

$Se_3(g)$

Selenium (ideal triatomic gas)

[Reaction: $1.5Se_2(g) = Se_3(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	$C_p°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta H°$	$\Delta G°$	
298.15	13.520	75.270	75.270	0	-7.850	-4.263	3.125
300	13.530	75.350	75.270	.025	-7.852	-4.240	3.089
400	13.860	79.300	75.805	1.398	-7.972	-3.020	1.650
500	14.050	82.420	76.832	2.794	-8.088	-1.770	.774
600	14.190	84.990	77.980	4.206	-8.192	-.497	.181
700	14.300	87.190	79.147	5.630	-8.283	.792	-.247
800	14.400	89.100	80.269	7.065	-8.360	2.104	-.575
900	14.490	90.800	81.346	8.509	-8.422	3.413	-.829
1000	14.570	92.330	82.368	9.962	-8.468	4.727	-1.033
1100	14.650	93.730	83.345	11.423	-8.498	6.044	-1.201
1200	14.730	95.000	84.257	12.892	-8.510	7.378	-1.344
1300	14.810	96.190	85.137	14.369	-8.508	8.697	-1.462
1400	14.890	97.290	85.966	15.854	-8.488	10.012	-1.563
1500	14.960	98.320	86.756	17.346	-8.453	11.332	-1.651
1600	15.040	99.280	87.501	18.846	-8.400	12.656	-1.729
1700	15.110	100.200	88.227	20.354	-8.331	13.982	-1.797
1800	15.190	101.060	88.911	21.869	-8.246	15.289	-1.856
1900	15.260	101.890	89.579	23.391	-8.144	16.575	-1.907
2000	15.340	102.670	90.209	24.921	-8.024	17.876	-1.953

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p° = 13.904 + 0.722\times10^{-3}T - 0.532\times10^{5}T^{-2}$

$H°- H°_{298} = 13.904\times10^{-3}T + 0.361\times10^{-6}T^2 + 0.532\times10^{2}T^{-1} - 4.356$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H° = -7.178 - 2.092\times10^{-3}T + 0.840\times10^{-6}T^2 - 36.650T^{-1}$

$\Delta G° = -7.178 + 2.092\times10^{-3}T\ln T - 0.840\times10^{-6}T^2 - 18.325T^{-1} - 1.687\times10^{-3}T$

Source: Data from Mills (158).

$Se_4(g)$

Selenium (ideal tetratomic gas)

[Reaction: $2Se_2(g) = Se_4(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	19.190	90.610	90.610	0	-22.800	-15.111	11.076
300	19.200	90.730	90.610	.036	-22.800	-15.063	10.973
400	19.490	96.310	91.375	1.974	-22.852	-12.480	6.819
500	19.620	100.670	92.810	3.930	-22.912	-9.877	4.317
600	19.700	104.260	94.433	5.896	-22.968	-7.272	2.649
700	19.740	107.290	96.050	7.868	-23.016	-4.641	1.449
800	19.770	109.930	97.625	9.844	-23.056	-2.008	.549
900	19.790	112.260	99.124	11.822	-23.086	.620	-.151
1000	19.800	114.350	100.548	13.802	-23.104	3.246	-.709
1100	19.820	116.240	101.892	15.783	-23.111	5.885	-1.169
1200	19.820	117.960	103.156	17.765	-23.105	8.527	-1.553
1300	19.830	119.550	104.360	19.747	-23.089	11.166	-1.877
1400	19.840	121.020	105.498	21.731	-23.059	13.789	-2.153
1500	19.840	122.390	106.580	23.715	-23.017	16.418	-2.392
1600	19.850	123.670	107.608	25.699	-22.963	19.037	-2.600
1700	19.850	124.870	108.585	27.684	-22.896	21.695	-2.789
1800	19.850	126.010	109.527	29.669	-22.817	24.289	-2.949
1900	19.850	127.080	110.420	31.654	-22.726	26.902	-3.094
2000	19.860	128.100	111.280	33.640	-22.620	29.500	-3.224

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.868 - 0.604\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.868\times10^{-3}T + 0.604\times10^{2}T^{-1} - 6.126$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = -22.222 - 1.460\times10^{-3}T + 0.638\times10^{-6}T^2 - 59.400T^{-1}$

$\Delta G^\circ = -22.222 + 1.460\times10^{-3}T\ln T - 0.638\times10^{-6}T^2 - 29.700T^{-1} + 16.058\times10^{-3}T$

Source: Data from Mills (158).

$Se_5(g)$

Selenium (ideal pentatomic gas)

[Reaction: $2.5Se_2(g) = Se_5(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	24.210	92.080	92.080	0	-50.250	-34.323	25.159
300	24.220	92.230	92.080	.045	-50.250	-34.224	24.932
400	24.920	99.320	93.045	2.510	-50.273	-28.881	15.779
500	25.240	104.920	94.880	5.020	-50.282	-23.530	10.285
600	25.410	109.540	96.950	7.554	-50.276	-18.185	6.624
700	25.520	113.470	99.040	10.101	-50.254	-12.836	4.007
800	25.590	116.880	101.059	12.657	-50.218	-7.482	2.044
900	25.640	119.900	102.991	15.218	-50.167	-2.152	.523
1000	25.670	122.600	104.816	17.784	-50.098	3.177	-.694
1100	25.700	125.050	106.547	20.353	-50.014	8.506	-1.690
1200	25.720	127.280	108.177	22.924	-49.914	13.831	-2.519
1300	25.740	129.340	109.727	25.497	-49.798	19.148	-3.219
1400	25.750	131.250	111.199	28.072	-49.665	24.430	-3.814
1500	25.760	133.030	112.599	30.647	-49.518	29.712	-4.329
1600	25.770	134.690	113.925	33.224	-49.354	34.982	-4.778
1700	25.780	136.250	115.190	35.802	-49.173	40.290	-5.180
1800	25.790	137.730	116.408	38.380	-48.978	45.513	-5.526
1900	25.790	139.120	117.563	40.959	-48.766	50.756	-5.838
2000	25.800	140.450	118.680	43.539	-48.536	55.964	-6.115

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 25.811 + 0.010\times10^{-3}T - 1.426\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.811\times10^{-3}T + 0.005\times10^{-6}T^2 + 1.426\times10^{2}T^{-1} - 8.174$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = -50.044 - 0.849\times10^{-3}T + 0.803\times10^{-6}T^2 - 7.150T^{-1}$

$\Delta G^\circ = -50.044 + 0.849\times10^{-3}T\ln T - 0.803\times10^{-6}T^2 - 3.575T^{-1} + 48.172\times10^{-3}T$

Source: Data from Mills (158).

$Se_6(g)$

Selenium (ideal hexatomic gas)

[Reaction: $3Se_2(g) = Se_6(G)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	30.180	103.610	103.610	0	-67.600	-46.434	34.037
300	30.190	103.800	103.613	.056	-67.598	-46.304	33.732
400	30.890	112.610	104.813	3.119	-67.520	-39.220	21.429
500	31.210	119.540	107.090	6.225	-67.438	-32.153	14.054
600	31.380	125.240	109.647	9.356	-67.340	-25.106	9.145
700	31.490	130.090	112.234	12.499	-67.227	-18.073	5.643
800	31.560	134.300	114.735	15.652	-67.098	-11.050	3.019
900	31.600	138.020	117.120	18.810	-66.952	-4.060	.986
1000	31.640	141.350	119.378	21.972	-66.787	2.913	-.637
1100	31.670	144.370	121.517	25.138	-66.603	9.880	-1.963
1200	31.690	147.120	123.532	28.305	-66.400	16.832	-3.065
1300	31.700	149.660	125.448	31.475	-66.179	23.768	-3.996
1400	31.720	152.010	127.263	34.646	-65.939	30.661	-4.786
1500	31.730	154.200	128.988	37.818	-65.680	37.550	-5.471
1600	31.740	156.250	130.631	40.991	-65.402	44.406	-6.066
1700	31.740	158.170	132.191	44.165	-65.105	51.311	-6.596
1800	31.750	159.990	133.691	47.339	-64.790	58.114	-7.056
1900	31.760	161.700	135.113	50.515	-64.455	64.935	-7.469
2000	31.760	163.330	136.484	53.691	-64.099	71.721	-7.837

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 31.778 + 0.008\times10^{-3}T - 1.422\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 31.778\times10^{-3}T + 0.004\times10^{-6}T^2 + 1.422\times10^{2}T^{-1} - 9.952$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = -67.496 - 0.214\times10^{-3}T + 0.961\times10^{-6}T^2 - 37.500T^{-1}$

$\Delta G^\circ = -67.496 + 0.214\times10^{-3}T\ln T - 0.961\times10^{-6}T^2 - 18.750T^{-1} + 69.919\times10^{-3}T$

Source: Data from Mills (158).

$Se_7(g)$

Selenium (ideal heptatomic gas)

[Reaction: $3.5Se_2(g) = Se_7(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	35.490	116.240	116.240	0	-82.150	-56.074	41.103
300	35.510	116.460	116.240	.066	-82.147	-55.912	40.731
400	36.480	126.850	117.658	3.677	-82.018	-47.190	25.783
500	36.930	135.040	120.340	7.350	-81.873	-38.496	16.826
600	37.170	141.800	123.373	11.056	-81.706	-29.845	10.871
700	37.320	147.540	126.423	14.782	-81.515	-21.206	6.621
800	37.420	152.530	129.381	18.519	-81.306	-12.594	3.440
900	37.490	156.940	132.202	22.264	-81.075	-4.026	.978
1000	37.540	160.890	134.874	26.016	-80.820	4.515	-.987
1100	37.570	164.470	137.405	29.771	-80.544	13.045	-2.592
1200	37.600	167.740	139.798	33.530	-80.243	21.542	-3.923
1300	37.620	170.750	142.065	37.291	-79.922	30.025	-5.048
1400	37.640	173.540	144.216	41.054	-79.578	38.449	-6.002
1500	37.660	176.140	146.261	44.819	-79.212	46.863	-6.828
1600	37.670	178.570	148.204	48.586	-78.823	55.241	-7.546
1700	37.680	180.860	150.064	52.354	-78.411	63.650	-8.183
1800	37.690	183.010	151.831	56.122	-77.979	71.971	-8.738
1900	37.700	185.050	153.528	59.892	-77.523	80.272	-9.233
2000	37.710	186.980	155.148	63.663	-77.042	88.558	-9.677

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 37.751 - 0.008\times10^{-3}T - 2.008\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 37.751\times10^{-3}T - 0.004\times10^{-6}T^2 + 2.008\times10^{2}T^{-1} - 11.929$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = -82.347 + 0.427\times10^{-3}T + 1.113\times10^{-6}T^2 - 8.850T^{-1}$

$\Delta G^\circ = -82.347 - 0.427\times10^{-3}T\ln T - 1.113\times10^{-6}T^2 - 4.425T^{-1} + 90.933\times10^{-3}T$

Source: Data from Mills (158).

$Se_8(g)$

Selenium (ideal octatomic gas)

[Reaction: $4Se_2(g) = Se_8(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	41.560	126.950	126.950	0	-96.200	-64.641	47.382
300	41.580	127.210	126.950	.078	-96.194	-64.445	46.948
400	42.510	139.340	128.605	4.294	-95.958	-53.902	29.450
500	42.930	148.870	131.732	8.569	-95.715	-43.410	18.974
600	43.170	156.720	135.262	12.875	-95.453	-32.981	12.013
700	43.310	163.390	138.820	17.199	-95.169	-22.586	7.052
800	43.400	169.180	142.262	21.534	-94.866	-12.226	3.340
900	43.460	174.290	145.537	25.878	-94.538	-1.919	.466
1000	43.510	178.880	148.653	30.227	-94.185	8.335	-1.822
1100	43.540	183.030	151.595	34.579	-93.809	18.578	-3.691
1200	43.570	186.820	154.374	38.935	-93.405	28.779	-5.241
1300	43.590	190.300	156.997	43.294	-92.978	38.972	-6.552
1400	43.610	193.530	159.491	47.654	-92.526	49.084	-7.662
1500	43.630	196.540	161.863	52.016	-92.048	59.182	-8.623
1600	43.640	199.360	164.123	56.379	-91.545	69.223	-9.455
1700	43.650	202.010	166.279	60.743	-91.017	79.306	-10.195
1800	43.660	204.500	168.328	65.109	-90.463	89.285	-10.841
1900	43.670	206.860	170.294	69.475	-89.885	99.241	-11.415
2000	43.670	209.100	172.179	73.842	-89.278	109.162	-11.929

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 43.735 - 0.024\times10^{-3}T - 1.927\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 43.735\times10^{-3}T - 0.012\times10^{-6}T^2 + 1.927\times10^{2}T^{-1} - 13.685$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = -96.477 + 1.079\times10^{-3}T + 1.264\times10^{-6}T^2 - 46.900T^{-1}$

$\Delta G^\circ = -96.477 - 1.079\times10^{-3}T\ln T - 1.264\times10^{-6}T^2 - 23.450T^{-1} + 113.567\times10^{-3}T$

Source: Data from Mills (158).

SeO(g)

Selenium Oxide (ideal gas)

[Formation: $Se(c,l) + 0.5O_2(g) = SeO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.466	55.923	55.923	0	12.750	6.406	-4.696
300	7.474	55.969	55.923	.014	12.747	6.367	-4.639
400	7.859	58.174	56.222	.781	12.543	4.271	-2.333
494.3	8.132	59.867	56.760	1.536	12.346	2.341	-1.035
494.3	8.132	59.867	56.760	1.536	10.874	2.341	-1.035
500	8.149	59.960	56.796	1.582	10.850	2.242	-.980
600	8.355	61.466	57.453	2.408	10.458	0.558	-.203
700	8.501	62.765	58.119	3.252	10.102	-1.062	.332
800	8.607	63.908	58.774	4.107	9.762	-2.635	.720
900	8.686	64.926	59.402	4.972	9.417	-4.164	1.011
958	8.721	65.470	59.753	5.477	9.209	-5.031	1.148

Phase changes: 494.3 K, melting point of Se; ΔH° = 1.472 kcal/mol.
958 K, boiling point of Se to equilibrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.254 + 0.510\times10^{-3}T - 0.836\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.254\times10^{-3}T + 0.255\times10^{-6}T^2 + 0.836\times10^{2}T^{-1} - 2.764$

Formation equations (kcal/mol):

298.15-494.3 K: $\Delta Hf^\circ = 12.950 - 0.823\times10^{-3}T - 1.181\times10^{-6}T^2 + 44.900T^{-1}$

$\Delta Gf^\circ = 12.950 + 0.823\times10^{-3}T\ln T + 1.181\times10^{-6}T^2 + 22.450T^{-1} - 27.240\times10^{-3}T$

494.3-958 K: $\Delta Hf^\circ = 11.030 - 1.795\times10^{-3}T - 0.625\times10^{-6}T^2 + 436.600T^{-1}$

$\Delta Gf^\circ = 11.030 + 1.795\times10^{-3}T\ln T + 0.625\times10^{-6}T^2 + 218.300T^{-1} - 29.912\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from Gordon (81).

SeO(g)

Selenium Oxide (ideal gas)

[Reaction: $0.5Se_2(g) + 0.5O_2(g) = SeO(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	$C_p°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta H°$	$\Delta G°$	
298.15	7.466	55.923	55.923	0	-3.900	-4.592	3.366
300	7.474	55.969	55.923	.014	-3.902	-4.596	3.348
400	7.859	58.174	56.222	.781	-3.987	-4.815	2.631
500	8.149	59.960	56.796	1.582	-4.055	-5.013	2.191
600	8.355	61.466	57.453	2.408	-4.113	-5.200	1.894
700	8.501	62.765	58.119	3.252	-4.162	-5.375	1.678
800	8.607	63.908	58.774	4.107	-4.210	-5.545	1.515
900	8.686	64.926	59.402	4.972	-4.254	-5.709	1.386
1000	8.747	65.845	60.001	5.844	-4.295	-5.871	1.283
1100	8.796	66.681	60.571	6.721	-4.335	-6.025	1.197
1200	8.835	67.448	61.112	7.603	-4.371	-6.176	1.125
1300	8.867	68.157	61.628	8.488	-4.406	-6.324	1.063
1400	8.894	68.815	62.118	9.376	-4.438	-6.473	1.010
1500	8.918	69.429	62.585	10.266	-4.468	-6.617	.964
1600	8.938	70.005	63.031	11.159	-4.497	-6.761	.924
1700	8.957	70.548	63.457	12.054	-4.522	-6.895	.886
1800	8.973	71.060	63.865	12.951	-4.546	-7.037	.854
1900	8.988	71.546	64.257	13.849	-4.568	-7.178	.826
2000	9.001	72.007	64.633	14.748	-4.588	-7.316	.799

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p° = 8.254 + 0.510\times10^{-3}T - 0.836\times10^{5}T^{-2}$

$H°- H°_{298} = 8.254\times10^{-3}T + 0.255\times10^{-6}T^{2} + 0.836\times10^{2}T^{-1} - 2.764$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H° = -3.812 - 0.693\times10^{-3}T + 0.163\times10^{-6}T^{2} + 31.050T^{-1}$

$\Delta G° = -3.812 + 0.693\times10^{-3}T\ln T - 0.163\times10^{-6}T^{2} + 15.525T^{-1} - 6.690\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from Gordon (81).

SeO_2(c,g)

Selenium Dioxide

[Formation: $Se(c,l) + O_2(g) = SeO_2(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.886	15.940	15.940	0	-53.860	-40.977	30.037
300	13.927	16.026	15.940	.026	-53.858	-40.897	29.793
400	15.825	20.306	16.511	1.518	-53.692	-36.598	19.996
494.3*	17.278	23.807	17.576	3.080	-53.425	-32.597	14.412
494.3	17.278	23.807	17.576	3.080	-54.897	-32.597	14.412
500	17.366	24.006	17.648	3.179	-54.890	-32.340	14.136
600	18.752	27.297	18.987	4.986	-54.678	-27.848	10.144
602	18.776	27.358	19.002	5.030	-54.666	-27.752	10.075
602	12.453	70.788	19.002	31.175	-28.521	-27.752	10.075
700	12.773	72.692	26.382	32.417	-28.837	-27.596	8.616
800	13.006	74.414	32.280	33.707	-29.141	-27.399	7.485
900	13.177	75.956	37.049	35.016	-29.448	-27.163	6.596
958	13.251	76.781	39.429	35.783	-29.634	-27.007	6.161

*Data estimated above 413 K to 602 K.

Phase changes: 494.3 K, melting point of Se; $\Delta H°$ = 1.472 kcal/mol.
602 K, sublimation point of SeO_2; $\Delta H°$ = 26.145 kcal/mol.
958 K, boiling point of Se to equilibrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-602 K: $Cp° = 11.292 + 13.152\times10^{-3}T - 1.180\times10^{5}T^{-2}$

$H°- H°_{298} = 11.292\times10^{-3}T + 6.576\times10^{-6}T^{2} + 1.180\times10^{2}T^{-1} - 4.347$

602.00-1500 K: $Cp° = 13.806 - 4.903\times10^{5}T^{-2}$

$H°- H°_{298} = 13.806\times10^{-3}T + 4.903\times10^{2}T^{-1} + 22.049$

Formation equations (kcal/mol):

298.15-494.3 K: $\Delta Hf° = -54.067 - 1.400\times10^{-3}T + 4.889\times10^{-6}T^{2} + 56.700T^{-1}$

$\Delta Gf° = -54.067 + 1.400\times10^{-3}T\ln T - 4.889\times10^{-6}T^{2} + 28.350T^{-1} + 37.067\times10^{-3}T$

494.3-602 K: $\Delta Hf° = -55.987 - 2.372\times10^{-3}T + 5.445\times10^{-6}T^{2} + 448.400T^{-1}$

$\Delta Gf° = -55.987 + 2.372\times10^{-3}T\ln T - 5.445\times10^{-6}T^{2} + 224.200T^{-1} + 34.394\times10^{-3}T$

602-958 K: $\Delta Hf° = -29.591 + 0.142\times10^{-3}T - 1.131\times10^{-6}T^{2} + 820.700T^{-1}$

$\Delta Gf° = -29.591 - 0.142\times10^{-3}T\ln T + 1.131\times10^{-6}T^{2} + 410.350T^{-1} + 2.164\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities and entropy at 298 K from Mal'stev (152). High-temperature data to 413 K based on Pashinkin (182) and estimated 413 to 602 K. Data for SeO_2(g) from Behrens (12).

$SeO_2(c,g)$

Selenium Dioxide

[Reaction: $0.5Se_2(g) + O_2(g) = SeO_2(c,g)$]

T, K	cal/mol•K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	13.886	15.940	15.940	0	-70.510	-51.976	38.099
300	13.927	16.026	15.940	.026	-70.506	-51.860	37.780
400	15.825	20.306	16.511	1.518	-70.221	-45.684	24.960
500*	17.366	24.006	17.648	3.179	-69.796	-39.596	17.307
600	18.752	27.297	18.987	4.986	-69.249	-33.606	12.241
602	18.776	27.358	19.002	5.030	-69.230	-33.480	12.154
602	12.453	70.788	19.002	31.175	-43.085	-33.480	12.154
700	12.773	72.692	26.382	32.417	-43.101	-31.909	9.962
800	13.006	74.414	32.280	33.707	-43.113	-30.308	8.280
900	13.177	75.956	37.049	35.016	-43.120	-28.708	6.971
1000	13.305	77.351	41.010	36.341	-43.122	-27.108	5.924
1100	13.403	78.624	44.373	37.676	-43.123	-25.505	5.067
1200	13.479	79.794	47.277	39.020	-43.121	-23.904	4.353
1300	13.540	80.875	49.820	40.371	-43.117	-22.300	3.749
1400	13.588	81.880	52.074	41.728	-43.112	-20.701	3.232
1500	13.628	82.819	54.093	43.089	-43.107	-19.101	2.783

*Data above 413 K to 602 K estimated.

Phase change: 602 K, sublimation point of SeO_2; ΔH° = 26.145 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-602 K:

$$Cp^\circ = 11.292 + 13.152\times10^{-3}T - 1.180\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 11.292\times10^{-3}T + 6.576\times10^{-6}T^2 + 1.180\times10^{2}T^{-1} - 4.347$$

602-1500 K:

$$Cp^\circ = 13.806 - 4.903\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 13.806\times10^{-3}T + 4.903\times10^{2}T^{-1} + 22.049$$

Reaction equations (kcal/mol):

298.15-602 K:

$$\Delta H^\circ = -70.829 - 1.270\times10^{-3}T + 6.232\times10^{-6}T^2 + 42.850T^{-1}$$

$$\Delta G^\circ = -70.829 + 1.270\times10^{-3}T\ln T - 6.232\times10^{-6}T^2 + 21.425T^{-1} + 57.617\times10^{-3}T$$

602-1500 K:

$$\Delta H^\circ = -44.433 + 1.244\times10^{-3}T - 0.343\times10^{-6}T^2 + 415.150T^{-1}$$

$$\Delta G^\circ = -44.433 - 1.244\times10^{-3}T\ln T + 0.343\times10^{-6}T^2 + 207.575T^{-1} + 25.387\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities and entropy at 298 K from Mal'stev (152). High-temperature data to 413 K based on Pashinkin (182) and estimated 413 to 602 K. Data for $SeO_2(g)$ from Behrens (12).

$SeO_2(g)$

Selenium Dioxide (ideal gas)

[Formation: $Se(c,l) + O_2(g) = SeO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.364	62.735	62.735	0	-26.200	-27.269	19.989
300	10.384	62.799	62.736	.019	-26.205	-27.276	19.870
400	11.309	65.919	63.154	1.106	-26.444	-27.596	15.077
494.3	11.942	68.382	63.923	2.204	-26.642	-27.847	12.312
494.3	11.942	68.382	63.923	2.204	-28.114	-27.847	12.312
500	11.980	68.519	63.975	2.272	-28.137	-27.844	12.170
600	12.446	70.747	64.922	3.495	-28.509	-27.749	10.108
700	12.773	72.692	65.896	4.757	-28.837	-27.596	8.616
800	13.006	74.414	66.855	6.047	-29.141	-27.399	7.485
900	13.177	75.956	67.783	7.356	-29.448	-27.163	6.596
958	13.251	76.781	68.302	8.123	-29.634	-27.007	6.161

Phase changes: 494.3 K, melting point of Se; $\Delta H° = 1.472$ kcal/mol.
958 K, boiling point of Se to equilibrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 12.030 + 1.390\times10^{-3}T - 1.849\times10^{5}T^{-2}$

$H°- H°_{298} = 12.030\times10^{-3}T + 0.695\times10^{-6}T^{2} + 1.849\times10^{2}T^{-1} - 4.269$

Formation equations (kcal/mol):

298.15-494.3 K: $\Delta Hf° = -26.329 - 0.662\times10^{-3}T - 0.992\times10^{-6}T^{2} + 123.600T^{-1}$

$\Delta Gf° = -26.329 + 0.662\times10^{-3}T\ln T + 0.992\times10^{-6}T^{2} + 61.800T^{-1} - 7.916\times10^{-3}T$

494.3-958 K: $\Delta Hf° = -28.249 - 1.634\times10^{-3}T - 0.436\times10^{-6}T^{2} + 515.300T^{-1}$

$\Delta Gf° = -28.249 + 1.634\times10^{-3}T\ln T + 0.436\times10^{-6}T^{2} + 257.650T^{-1} - 10.588\times10^{-3}T$

Source: Data from Behrens (12).

$SeO_2(g)$

Selenium Dioxide (ideal gas)

[Reaction: $0.5Se_2(g) + O_2(g) = SeO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	10.364	62.735	62.735	0	-42.850	-38.267	28.050
300	10.384	62.799	62.736	.019	-42.853	-38.239	27.857
400	11.309	65.919	63.154	1.106	-42.974	-36.681	20.041
500	11.980	68.519	63.975	2.272	-43.043	-35.099	15.342
600	12.446	70.747	64.922	3.495	-43.080	-33.507	12.205
700	12.773	72.692	65.896	4.757	-43.101	-31.909	9.962
800	13.006	74.414	66.855	6.047	-43.113	-30.308	8.280
900	13.177	75.956	67.783	7.356	-43.120	-28.708	6.971
1000	13.305	77.351	68.670	8.681	-43.122	-27.108	5.924
1100	13.403	78.624	69.519	10.016	-43.123	-25.505	5.067
1200	13.479	79.794	70.327	11.360	-43.121	-23.904	4.353
1300	13.540	80.875	71.097	12.711	-43.117	-22.300	3.749
1400	13.588	81.880	71.831	14.068	-43.112	-20.701	3.232
1500	13.628	82.819	72.533	15.429	-43.107	-19.101	2.783

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 12.030 + 1.390\times10^{-3}T - 1.849\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 12.030\times10^{-3}T + 0.695\times10^{-6}T^2 + 1.849\times10^{2}T^{-1} - 4.269$

Reaction equations (kcal/mol):

298.15-1500 K: $\Delta H^\circ = -43.091 - 0.532\times10^{-3}T + 0.352\times10^{-6}T^2 + 109.750T^{-1}$

$\Delta G^\circ = -43.091 + 0.532\times10^{-3}T\ln T - 0.352\times10^{-6}T^2 + 54.875T^{-1} + 12.634\times10^{-3}T$

Source: Data from Behrens (12).

Si(c,l)

Silicon

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	4.780	4.500	4.500	0
300	4.790	4.530	4.500	.009
400	5.300	5.980	4.690	.516
500	5.610	7.200	5.076	1.062
600	5.820	8.240	5.517	1.634
700	5.990	9.150	5.971	2.225
800	6.130	9.960	6.423	2.830
900	6.240	10.690	6.857	3.450
1000	6.330	11.360	7.282	4.078
1100	6.410	11.960	7.674	4.715
1200	6.470	12.520	8.054	5.359
1300	6.530	13.040	8.418	6.009
1400	6.600	13.530	8.769	6.666
1500	6.650	13.980	9.094	7.329
1600	6.710	14.410	9.412	7.997
1687	6.770	14.780	9.691	8.583
1687	6.100	21.940	9.691	20.665
1700	6.100	21.990	9.788	20.744
1800	6.100	22.340	10.477	21.354
1900	6.100	22.670	11.110	21.964
2000	6.100	22.980	11.693	22.574

Phase changes: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.
3540 K, boiling point of Si to equilibrium mixture of Si(g), Si_2(g), and Si_3(g).

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1687 K: $Cp^\circ = 5.679 + 0.702\times10^{-3}T - 0.985\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.679\times10^{-3}T + 0.351\times10^{-6}T^2 + 0.985\times10^{2}T^{-1} - 2.055$

1687-2000 K: $Cp^\circ = 6.100$

$H^\circ - H^\circ_{298} = 6.100\times10^{-3}T + 10.374$

Source: Data from Hultgren (99) corrected to IPTS-68.

Si(g)

Silicon (ideal monatomic gas)

[Formation: Si(c,1) = Si(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.318	40.121	40.121	0	107.700	97.080	-71.160
300	5.314	40.154	40.121	.010	107.701	97.014	-70.674
400	5.166	41.660	40.327	.533	107.717	93.445	-51.055
500	5.095	42.804	40.714	1.045	107.683	89.881	-39.286
600	5.056	43.729	41.141	1.553	107.619	86.326	-31.444
700	5.033	44.506	41.567	2.057	107.532	82.783	-25.846
800	5.019	45.178	41.978	2.560	107.430	79.256	-21.651
900	5.012	45.768	42.367	3.061	107.311	75.741	-18.392
1000	5.011	46.296	42.734	3.562	107.184	72.248	-15.790
1100	5.016	46.774	43.079	4.064	107.049	68.754	-13.660
1200	5.027	47.211	43.406	4.566	106.907	65.278	-11.889
1300	5.043	47.614	43.715	5.069	106.760	61.814	-10.392
1400	5.063	47.988	44.007	5.574	106.608	58.367	-9.111
1500	5.087	48.338	44.283	6.082	106.453	54.916	-8.001
1600	5.113	48.668	44.548	6.592	106.295	51.482	-7.032
1687	5.138	48.939	44.767	7.038	106.155	48.529	-6.287
1687	5.138	48.939	44.767	7.038	94.073	48.529	-6.287
1700	5.142	48.978	44.799	7.105	94.061	48.181	-6.194
1800	5.171	49.273	45.040	7.620	93.966	45.487	-5.523
1900	5.202	49.553	45.269	8.139	93.875	42.797	-4.923
2000	5.232	49.821	45.491	8.660	93.786	40.104	-4.382

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.845 + 0.154\times10^{-3}T + 0.380\times10^{5}T^{-2}$

$H°- H°_{298} = 4.845\times10^{-3}T + 0.077\times10^{-6}T^{2} - 0.380\times10^{2}T^{-1} - 1.324$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = 108.431 - 0.834\times10^{-3}T - 0.274\times10^{-6}T^{2} - 136.500T^{-1}$

$\Delta Gf° = 108.431 + 0.834\times10^{-3}T\ln T + 0.274\times10^{-6}T^{2} - 68.250T^{-1} - 42.138\times10^{-3}T$

1687-2000 K: $\Delta Hf° = 96.002 - 1.255\times10^{-3}T + 0.077\times10^{-6}T^{2} - 38.000T^{-1}$

$\Delta Gf° = 96.002 + 1.255\times10^{-3}T\ln T - 0.077\times10^{-6}T^{2} - 19.000T^{-1} - 37.324\times10^{-3}T$

Source: Data from JANAF (51).

$Si_2(g)$

Silicon (ideal diatomic gas)

[Formation: $2Si(c,l) = Si_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.234	54.895	54.895	0	141.000	127.316	-93.324
300	8.242	54.946	54.896	.015	140.997	127.231	-92.687
400	8.658	57.375	55.222	.861	140.829	122.663	-67.019
500	9.079	59.352	55.858	1.747	140.623	118.147	-51.641
600	9.499	61.045	56.585	2.676	140.408	113.669	-41.403
700	9.867	62.537	57.330	3.645	140.195	109.229	-34.102
800	10.151	63.875	58.066	4.647	139.987	104.823	-28.636
900	10.343	65.082	58.780	5.672	139.772	100.440	-24.390
1000	10.453	66.178	59.465	6.713	139.557	96.099	-21.002
1100	10.502	67.177	60.122	7.761	139.331	91.748	-18.228
1200	10.507	68.091	60.748	8.812	139.094	87.433	-15.923
1300	10.485	68.932	61.347	9.861	138.843	83.135	-13.976
1400	10.447	69.707	61.916	10.908	138.576	78.870	-12.312
1500	10.401	70.427	62.460	11.951	138.293	74.592	-10.868
1600	10.354	71.096	62.979	12.988	137.994	70.352	-9.610
1687	10.315	71.644	63.412	13.888	137.722	66.723	-8.644
1687	10.315	71.644	63.412	13.888	113.558	66.723	-8.644
1700	10.309	71.723	63.475	14.022	113.534	66.371	-8.532
1800	10.268	72.311	63.950	15.050	113.342	63.606	-7.723
1900	10.232	72.865	64.404	16.075	113.147	60.849	-6.999
2000	10.200	73.389	64.840	17.097	112.949	58.091	-6.348

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.703 + 0.534\times10^{-3}T - 1.448\times10^{5}T^{-2}$

$H°- H°_{298} = 9.703\times10^{-3}T + 0.267\times10^{-6}T^{2} + 1.448\times10^{2}T^{-1} - 3.402$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = 141.707 - 1.655\times10^{-3}T - 0.435\times10^{-6}T^{2} - 52.200T^{-1}$

$\Delta Gf° = 141.707 + 1.655\times10^{-3}T\ln T + 0.435\times10^{-6}T^{2} - 26.100T^{-1} - 57.533\times10^{-3}T$

1687-2000 K: $\Delta Hf° = 116.849 - 2.497\times10^{-3}T + 0.267\times10^{-6}T^{2} + 144.800T^{-1}$

$\Delta Gf° = 116.849 + 2.497\times10^{-3}T\ln T - 0.267\times10^{-6}T^{2} + 72.400T^{-1} - 47.904\times10^{-3}T$

Source: Data from JANAF (51).

$Si_3(g)$

Silicon (ideal triatomic gas)

[Formation: $3Si(c,l) = Si_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.158	64.002	64.002	0	152.000	136.943	-100.381
300	13.174	64.084	64.004	.024	151.997	136.849	-99.693
400	13.811	67.971	64.529	1.377	151.829	131.817	-72.020
500	14.162	71.094	65.540	2.777	151.591	126.844	-55.443
600	14.371	73.696	66.688	4.205	151.303	121.917	-44.408
700	14.504	75.922	67.852	5.649	150.974	117.044	-36.542
800	14.594	77.865	68.985	7.104	150.614	112.226	-30.658
900	14.656	79.587	70.068	8.567	150.217	107.452	-26.093
1000	14.702	81.134	71.099	10.035	149.801	102.747	-22.455
1100	14.738	82.537	72.076	11.507	149.362	98.039	-19.478
1200	14.766	83.821	73.003	12.982	148.905	93.392	-17.009
1300	14.790	85.004	73.881	14.460	148.433	88.784	-14.926
1400	14.814	86.101	74.715	15.940	147.942	84.227	-13.148
1500	14.838	87.123	75.508	17.423	147.436	79.662	-11.607
1600	14.863	88.082	76.265	18.908	146.917	75.154	-10.265
1687	14.889	88.870	76.894	20.202	146.453	71.328	-9.240
1687	14.889	88.870	76.894	20.202	110.207	71.328	-9.240
1700	14.893	88.984	76.986	20.396	110.164	71.040	-9.133
1800	14.926	89.836	77.677	21.886	109.824	68.755	-8.348
1900	14.964	90.644	78.338	23.381	109.489	66.484	-7.647
2000	15.007	91.413	78.974	24.879	109.157	64.211	-7.017

*All data except enthalpy of formation at 298 K estimated.

Phase change: 1687 K; melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.624 + 0.192\times10^{-3}T - 1.354\times10^{5}T^{-2}$

$H°- H°_{298} = 14.624\times10^{-3}T + 0.096\times10^{-6}T^{2} + 1.354\times10^{2}T^{-1} - 4.823$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = 153.341 - 2.413\times10^{-3}T - 0.957\times10^{-6}T^{2} - 160.100T^{-1}$

$\Delta Gf° = 153.341 + 2.413\times10^{-3}T\ln T + 0.957\times10^{-6}T^{2} - 80.050T^{-1} - 68.134\times10^{-3}T$

1687-2000 K: $\Delta Hf° = 116.054 - 3.676\times10^{-3}T + 0.096\times10^{-6}T^{2} + 135.400T^{-1}$

$\Delta Gf° = 116.054 + 3.676\times10^{-3}T\ln T - 0.096\times10^{-6}T^{2} + 67.700T^{-1} - 53.692\times10^{-3}T$

Source: Data from JANAF (51) who estimated all except enthalpy of formation at 298 K.

SiO(g)

Silicon Monoxide (ideal gas)

[Formation: $Si(c,1) + 0.5O_2(g) = SiO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.146	50.542	50.542	0	-23.800	-30.222	22.153
300	7.151	50.586	50.543	.013	-23.802	-30.262	22.046
400	7.441	52.682	50.827	.742	-23.935	-32.398	17.701
500	7.735	54.374	51.370	1.502	-24.087	-34.494	15.077
600	7.982	55.807	51.994	2.288	-24.250	-36.562	13.317
700	8.177	57.053	52.630	3.096	-24.422	-38.601	12.052
800	8.328	58.155	53.252	3.922	-24.601	-40.612	11.095
900	8.445	59.143	53.853	4.761	-24.788	-42.603	10.345
1000	8.538	60.038	54.428	5.610	-24.981	-44.564	9.739
1100	8.611	60.855	54.975	6.468	-25.179	-46.519	9.242
1200	8.671	61.607	55.497	7.332	-25.384	-48.451	8.824
1300	8.720	62.303	55.995	8.201	-25.592	-50.366	8.467
1400	8.761	62.951	56.469	9.075	-25.808	-52.260	8.158
1500	8.795	63.556	56.921	9.953	-26.028	-54.152	7.890
1600	8.825	64.125	57.354	10.834	-26.253	-56.022	7.652
1687	8.847	64.593	57.715	11.603	-26.454	-57.614	7.464
1687	8.847	64.593	57.715	11.603	-38.536	-57.614	7.464
1700	8.850	64.661	57.768	11.718	-38.557	-57.757	7.425
1800	8.873	65.167	58.165	12.604	-38.725	-58.878	7.149
1900	8.893	65.648	58.546	13.493	-38.893	-59.993	6.901
2000	8.911	66.104	58.912	14.383	-39.062	-61.104	6.677

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.807 + 0.684\times10^{-3}T - 0.769\times10^{5}T^{-2}$

$H°- H°_{298} = 7.807\times10^{-3}T + 0.342\times10^{-6}T^{2} + 0.769\times10^{2}T^{-1} - 2.616$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -23.185 - 1.487\times10^{-3}T - 0.260\times10^{-6}T^{2} - 44.200T^{-1}$

$\Delta Gf° = -23.185 + 1.487\times10^{-3}T\ln T + 0.260\times10^{-6}T^{2} - 22.100T^{-1} - 31.903\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -35.614 - 1.908\times10^{-3}T + 0.091\times10^{-6}T^{2} + 54.300T^{-1}$

$\Delta Gf° = -35.614 + 1.908\times10^{-3}T\ln T - 0.091\times10^{-6}T^{2} + 27.150T^{-1} - 27.089\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data from JANAF (51).

SiO_2(quartz)

Silicon Dioxide

[Formation: $Si(c,l) + O_2(g) = SiO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.620	10.000	10.000	0	-217.720	-204.749	150.083
300	10.664	10.066	10.000	.020	-217.722	-204.668	149.099
400	12.732	13.431	10.443	1.195	-217.764	-200.308	109.442
500	14.247	16.444	11.348	2.548	-217.688	-195.950	85.648
600	15.385	19.146	12.428	4.031	-217.532	-191.617	69.796
700	16.438	21.596	13.565	5.622	-217.310	-187.315	58.482
800	17.920	23.875	14.712	7.330	-217.005	-183.049	50.006
847	21.700	24.970	15.254	8.230	-216.775	-181.063	46.719
847	16.631	25.177	15.254	8.405	-216.600	-181.063	46.719
900	16.666	26.187	15.867	9.288	-216.481	-178.841	43.428
1000	16.733	27.947	16.989	10.958	-216.266	-174.663	38.172
1100	16.800	29.544	18.058	12.635	-216.065	-170.518	33.878
1200	16.867	31.009	19.077	14.318	-215.874	-166.387	30.303
1300	16.934	32.362	20.048	16.008	-215.690	-162.272	27.280
1400	17.001	33.619	20.973	17.705	-215.514	-158.164	24.690
1500	17.067	34.794	21.855	19.408	-215.344	-154.085	22.450
1600	17.134	35.898	22.699	21.118	-215.179	-150.009	20.490
1687	17.192	36.807	23.404	22.611	-215.039	-146.448	18.972
1687	17.192	36.807	23.404	22.611	-227.121	-146.448	18.972
1700	17.201	36.939	23.507	22.835	-227.091	-145.823	18.747
1800	17.268	37.924	24.280	24.559	-226.865	-141.045	17.125
1900	17.335	38.859	25.023	26.289	-226.639	-136.283	15.676
2000	17.402	39.750	25.737	28.026	-226.411	-131.539	14.374

Phase changes: 847 K, α ~ β (low - high) transition point of quartz; $\Delta H° = 0.175$ kcal/mol.
1100 K, quartz to cristobalite transition point; $\Delta H° = 0.5$ kcal/mol.
Temperature and enthalpy not well defined. Quartz is metastable above this transition.
1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.
1700 K, melting point of metastable quartz; $\Delta H° = 2$ kcal/mol.
Temperature and enthalpy of fusion not well defined. Quartz may be superheated above this temperature.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-847 K:
$$Cp° = 9.679 + 10.660\times10^{-3}T - 1.989\times10^{5}T^{-2}$$
$$H°- H°_{298} = 9.679\times10^{-3}T + 5.330\times10^{-6}T^{2} + 1.989\times10^{2}T^{-1} - 4.027$$

847-2000 K:
$$Cp° = 16.155 + 0.616\times10^{-3}T - 0.326\times10^{5}T^{-2}$$
$$H°- H°_{298} = 16.155\times10^{-3}T + 0.308\times10^{-6}T^{2} + 0.326\times10^{2}T^{-1} - 5.538$$

Formation equations (kcal/mol):

298.15-847 K:
$$\Delta Hf° = -217.340 - 3.230\times10^{-3}T + 4.476\times10^{-6}T^{2} + 55.200T^{-1}$$
$$\Delta Gf° = -217.340 + 3.230\times10^{-3}T\ln T - 4.476\times10^{-6}T^{2} + 27.600T^{-1} + 24.851\times10^{-3}T$$

847-1687 K:
$$\Delta Hf° = -218.851 + 3.246\times10^{-3}T - 0.546\times10^{-6}T^{2} - 111.100T^{-1}$$
$$\Delta Gf° = -218.851 - 3.246\times10^{-3}T\ln T + 0.546\times10^{-6}T^{2} - 55.550T^{-1} + 66.157\times10^{-3}T$$

1687-2000 K:
$$\Delta Hf° = -231.280 + 2.825\times10^{-3}T - 0.195\times10^{-6}T^{2} - 12.600T^{-1}$$
$$\Delta Gf° = -231.280 - 2.825\times10^{-3}T\ln T + 0.195\times10^{-6}T^{2} - 6.300T^{-1} + 70.971\times10^{-3}T$$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (236). Low-temperature heat capacities from Anderson (6). High-temperature data based on Moser (162), Roth (191), White (249), and Wietzel (251).

SiO_2(cristobalite)

Silicon Dioxide

[Formation: $Si(c,l) + O_2(g) = SiO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.693	10.200	10.200	0	-217.370	-204.459	149.870
300	10.740	10.266	10.200	.020	-217.372	-204.378	148.887
400	12.697	13.647	10.647	1.200	-217.409	-200.040	109.295
500	14.051	16.632	11.552	2.540	-217.346	-195.702	85.540
543	14.551	17.812	12.002	3.155	-217.296	-193.842	78.018
543	14.787	18.383	12.002	3.465	-216.986	-193.842	78.018
600	15.193	19.880	12.680	4.320	-216.893	-191.419	69.723
700	15.711	22.263	13.882	5.867	-216.715	-187.187	58.442
800	16.083	24.386	15.065	7.457	-216.528	-182.981	49.987
900	16.369	26.298	16.209	9.080	-216.339	-178.799	43.418
1000	16.602	28.035	17.306	10.729	-216.145	-174.630	38.165
1100	16.800	29.627	18.354	12.400	-215.950	-170.495	33.874
1200	16.975	31.096	19.355	14.089	-215.753	-166.371	30.300
1300	17.133	32.461	20.312	15.794	-215.554	-162.264	27.279
1400	17.279	33.737	21.226	17.515	-215.354	-158.170	24.691
1500	17.416	34.933	22.100	19.250	-215.152	-154.102	22.452
1600	17.547	36.062	22.938	20.998	-214.949	-150.042	20.494
1687	17.656	36.993	23.639	22.529	-214.771	-146.494	18.978
1687	17.656	36.993	23.639	22.529	-226.853	-146.494	18.978
1700	17.672	37.129	23.741	22.759	-226.817	-145.871	18.753
1800	17.793	38.143	24.514	24.532	-226.542	-141.116	17.134
1900	17.910	39.108	25.257	26.317	-226.261	-136.378	15.687
2000	18.025	40.029	25.972	28.114	-225.973	-131.659	14.387

Phase changes: 543 K, α - β (low - high) transition point of cristobalite; $\Delta H° = 0.310$ kcal/mol.
1100 K, quartz to cristobalite transition point; $\Delta H° = 0.5$ kcal/mol.
Temperature and enthalpy of transition not well defined. Cristobalite is metastable below this transition.
1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.
2000 K, melting point of cristobalite; $\Delta H° = 2$ kcal/mol.
Temperature and enthalpy of fusion not well defined.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-543 K:

$$Cp° = 10.814 + 8.324\times10^{-3}T - 2.313\times10^{5}T^{-2}$$

$$H°- H°_{298} = 10.814\times10^{-3}T + 4.162\times10^{-6}T^{2} + 2.313\times10^{2}T^{-1} - 4.370$$

543-2000 K:

$$Cp° = 16.167 + 1.002\times10^{-3}T - 5.672\times10^{5}T^{-2}$$

$$H°- H°_{298} = 16.167\times10^{-3}T + 0.501\times10^{-6}T^{2} + 5.672\times10^{2}T^{-1} - 6.506$$

Formation equations (kcal/mol):

298.15-543 K:

$$\Delta Hf° = -217.333 - 2.095\times10^{-3}T + 3.308\times10^{-6}T^{2} + 87.600T^{-1}$$

$$\Delta Gf° = -217.333 + 2.095\times10^{-3}T\ln T - 3.308\times10^{-6}T^{2} + 43.800T^{-1} + 31.739\times10^{-3}T$$

543-1687 K:

$$\Delta Hf° = -219.469 + 3.258\times10^{-3}T - 0.353\times10^{-6}T^{2} + 423.500T^{-1}$$

$$\Delta Gf° = -219.469 - 3.258\times10^{-3}T\ln T + 0.353\times10^{-6}T^{2} + 211.750T^{-1} + 66.823\times10^{-3}T$$

1687-2000 K:

$$\Delta Hf° = -231.898 + 2.837\times10^{-3}T - 0.002\times10^{-6}T^{2} + 522.000T^{-1}$$

$$\Delta Gf° = -231.898 - 2.837\times10^{-3}T\ln T + 0.002\times10^{-6}T^{2} + 261.000T^{-1} + 71.637\times10^{-3}T$$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (236). Low-temperature heat capacities from Anderson (6). High-temperature data based on Mosesman (163), White (249), and Wietzel (251). Temperature of low-high transition from Walker (241).

SiO_2(tridymite)

Silicon Dioxide

[Formation: $Si(c,l) + O_2(g) = SiO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.660	10.360	10.360	0	-217.270	-204.406	149.832
300	10.705	10.426	10.360	.020	-217.272	-204.326	148.850
390	12.913	13.519	10.737	1.085	-217.299	-200.438	112.321
390	13.403	13.647	10.737	1.135	-217.249	-200.438	112.321
400	13.495	13.988	10.816	1.269	-217.240	-200.007	109.277
500	14.415	17.099	11.769	2.665	-217.121	-195.710	85.544
500	14.089	17.189	11.769	2.710	-217.076	-195.710	85.544
600	15.100	19.855	12.898	4.174	-216.939	-191.450	69.735
700	15.709	22.232	14.065	5.717	-216.765	-187.215	58.450
800	16.110	24.358	15.220	7.310	-216.575	-183.005	49.994
900	16.396	26.273	16.344	8.936	-216.383	-178.821	43.423
1000	16.615	28.012	17.425	10.587	-216.187	-174.649	38.169
1100	16.796	29.604	18.461	12.257	-215.993	-170.512	33.877
1200	16.955	31.073	19.452	13.945	-215.797	-166.387	30.303
1300	17.102	32.436	20.399	15.648	-215.600	-162.278	27.281
1400	17.245	33.708	21.304	17.365	-215.404	-158.179	24.693
1500	17.388	34.903	22.172	19.097	-215.205	-154.110	22.454
1600	17.534	36.030	23.003	20.843	-215.004	-150.046	20.495
1687	17.666	36.961	23.699	22.374	-214.826	-146.495	18.978
1687	17.666	36.961	23.699	22.374	-226.908	-146.495	18.978
1700	17.686	37.097	23.801	22.604	-226.872	-145.872	18.753
1800	17.846	38.113	24.569	24.380	-226.594	-141.114	17.133
1900	18.014	39.082	25.307	26.173	-226.305	-136.372	15.686
2000	18.193	40.011	26.019	27.984	-226.003	-131.653	14.386

Phase changes: 390 K, transition point of tridymite; $\Delta H° = 0.050$ kcal/mol.
500 K, transition point of tridymite; $\Delta H° = 0.045$ kcal/mol.
1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-390 K: $Cp° = 3.373 + 24.530\times10^{-3}T$

$H°- H°_{298} = 3.373\times10^{-3}T + 12.265\times10^{-6}T^2 - 2.096$

390-500 K: $Cp° = 9.816 + 9.200\times10^{-3}T$

$H°- H°_{298} = 9.816\times10^{-3}T + 4.600\times10^{-6}T^2 - 3.393$

500-2000 K: $Cp° = 16.812 + 0.606\times10^{-3}T - 7.567\times10^{5}T^{-2}$

$H°- H°_{298} = 16.812\times10^{-3}T + 0.303\times10^{-6}T^2 + 7.567\times10^{2}T^{-1} - 7.285$

Formation equations (kcal/mol):

298.15-390 K: $\Delta Hf° = -214.959 - 9.536\times10^{-3}T + 11.411\times10^{-6}T^2 - 143.700T^{-1}$

$\Delta Gf° = -214.959 + 9.536\times10^{-3}T\ln T - 11.411\times10^{-6}T^2 - 71.850T^{-1} - 14.727\times10^{-3}T$

390-500 K: $\Delta Hf° = -216.256 - 3.093\times10^{-3}T + 3.746\times10^{-6}T^2 - 143.700T^{-1}$

$\Delta Gf° = -216.256 + 3.093\times10^{-3}T\ln T - 3.746\times10^{-6}T^2 - 71.850T^{-1} + 24.049\times10^{-3}T$

500-1687 K: $\Delta Hf° = -220.148 + 3.903\times10^{-3}T - 0.551\times10^{-6}T^2 + 613.000T^{-1}$

$\Delta Gf° = -220.148 - 3.903\times10^{-3}T\ln T + 0.551\times10^{-6}T^2 + 306.500T^{-1} + 71.649\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -232.577 + 3.482\times10^{-3}T - 0.200\times10^{-6}T^2 + 711.500T^{-1}$

$\Delta Gf° = -232.577 - 3.482\times10^{-3}T\ln T + 0.200\times10^{-6}T^2 + 355.750T^{-1} + 76.463\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities and entropy at 298 K from Anderson (6). High-temperature data based on Mosesman (163).

SiO_2(vitreous)

Silicon Dioxide, Silica Glass

[Formation: $Si(c,l) + O_2(g) = SiO_2(vit)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.600	11.200	11.200	0	-215.940	-203.327	149.041
300	10.642	11.266	11.200	.020	-215.942	-203.248	148.064
400	12.529	14.595	11.640	1.182	-215.997	-199.007	108.731
500	13.922	17.549	12.533	2.508	-215.948	-194.762	85.129
600	14.918	20.181	13.593	3.953	-215.830	-190.536	69.402
700	15.619	22.536	14.705	5.482	-215.670	-186.333	58.175
800	16.109	24.656	15.819	7.070	-215.485	-182.154	49.761
900	16.461	26.574	16.908	8.699	-215.290	-177.998	43.223
1000	16.738	28.323	17.964	10.359	-215.085	-173.858	37.996
1100	16.991	29.931	18.980	12.046	-214.874	-169.753	33.726
1200	17.261	31.420	19.955	13.758	-214.654	-165.660	30.170
1300	17.579	32.814	20.892	15.499	-214.419	-161.588	27.165
1400	17.966	34.130	21.790	17.276	-214.163	-157.529	24.591
1500	18.434	35.385	22.655	19.095	-213.877	-153.505	22.365
1600	18.983	36.592	23.488	20.966	-213.551	-149.492	20.419
1687	19.523	37.611	24.191	22.640	-213.230	-145.996	18.914
1687	19.523	37.611	24.191	22.640	-225.312	-145.996	18.914
1700	19.604	37.761	24.294	22.894	-225.252	-145.381	18.690
1800	20.277	38.901	25.074	24.888	-224.756	-140.694	17.082
1900	20.974	40.016	25.831	26.951	-224.197	-136.039	15.648
2000	21.655	41.109	26.568	29.082	-223.575	-131.421	14.361

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.647 + 3.474\times10^{-3}T - 3.629\times10^{5}T^{-2}$

$H°- H°_{298} = 13.647\times10^{-3}T + 1.737\times10^{-6}T^{2} + 3.629\times10^{2}T^{-1} - 5.440$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -216.974 + 0.738\times10^{-3}T + 0.883\times10^{-6}T^{2} + 219.200T^{-1}$

$\Delta Gf° = -216.974 - 0.738\times10^{-3}T\ln T - 0.883\times10^{-6}T^{2} + 109.600T^{-1} + 49.007\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -229.403 + 0.317\times10^{-3}T + 1.234\times10^{-6}T^{2} + 317.700T^{-1}$

$\Delta Gf° = -229.403 - 0.317\times10^{-3}T\ln T - 1.234\times10^{-6}T^{2} + 158.850T^{-1} + 53.821\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (236). Low-temperature heat capacities based on Simon (202) and Kelley (122). High-temperature data based on Ferrante (60), Wietzel (251), and Shmidt (196).

$SiO_2(g)$

Silicon Dioxide (ideal gas)

[Formation: $Si(c,l) + O_2(g) = SiO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	10.518	54.699	54.699	0	-77.000	-77.356	56.703
300	10.537	54.765	54.702	.019	-77.003	-77.359	56.355
400	11.474	57.929	55.124	1.122	-77.117	-77.461	42.322
500	12.207	60.572	55.958	2.307	-77.209	-77.534	33.890
600	12.767	62.849	56.921	3.557	-77.286	-77.593	28.263
700	13.188	64.851	57.914	4.856	-77.356	-77.639	24.240
800	13.507	66.633	58.893	6.192	-77.423	-77.673	21.219
900	13.750	68.239	59.845	7.555	-77.494	-77.701	18.868
1000	13.938	69.698	60.758	8.940	-77.564	-77.712	16.984
1100	14.085	71.033	61.632	10.341	-77.639	-77.730	15.443
1200	14.203	72.264	62.467	11.756	-77.716	-77.735	14.157
1300	14.297	73.405	63.266	13.181	-77.797	-77.735	13.068
1400	14.374	74.467	64.028	14.615	-77.884	-77.722	12.133
1500	14.438	75.461	64.758	16.055	-77.977	-77.719	11.324
1600	14.491	76.395	65.456	17.502	-78.075	-77.701	10.613
1687	14.530	77.163	66.041	18.764	-78.166	-77.656	10.060
1687	14.530	77.163	66.041	18.764	-90.248	-77.656	10.060
1700	14.536	77.275	66.126	18.953	-90.253	-77.556	9.970
1800	14.573	78.107	66.769	20.409	-90.295	-76.804	9.325
1900	14.606	78.896	67.387	21.868	-90.340	-76.054	8.748
2000	14.634	79.645	67.980	23.330	-90.387	-75.305	8.229

*All data except enthalpy of formation at 298 K estimated.

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.501 + 1.418\times10^{-3}T - 2.138\times10^{5}T^{-2}$

$H°- H°_{298} = 12.501\times10^{-3}T + 0.709\times10^{-6}T^{2} + 2.138\times10^{2}T^{-1} - 4.507$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -77.101 - 0.408\times10^{-3}T - 0.145\times10^{-6}T^{2} + 70.100T^{-1}$

$\Delta Gf° = -77.101 + 0.408\times10^{-3}T\ln T + 0.145\times10^{-6}T^{2} + 35.050T^{-1} - 3.619\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -89.530 - 0.829\times10^{-3}T + 0.206\times10^{-6}T^{2} + 168.600T^{-1}$

$\Delta Gf° = -89.530 + 0.829\times10^{-3}T\ln T - 0.206\times10^{-6}T^{2} + 84.300T^{-1} + 1.195\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). All other data are those estimated by JANAF (51).

Sm(c,1)

Samarium

T, K	cal/mol·K			$H°- H^{\circ}_{298}$,
	$Cp°$	$S°$	$-(G°- H^{\circ}_{298})/T$	kcal/mol
298.15	7.060	16.630	16.630	0
300	7.080	16.670	16.630	.013
400	7.930	18.810	16.913	.759
500	8.940	20.700	17.490	1.605
600	9.750	22.400	18.163	2.542
700	10.190	23.950	18.887	3.544
800	10.520	25.330	19.609	4.577
900	10.630	26.580	20.314	5.639
1000	10.820	27.710	21.000	6.710
1100	11.120	28.750	21.650	7.810
1190	11.560	29.640	22.222	8.831
1190	11.220	30.270	22.222	9.575
1200	11.220	30.370	22.298	9.687
1300	11.220	31.260	22.945	10.809
1345	11.220	31.650	23.238	11.314
1345*	12.000	33.180	23.238	13.374
1400	12.000	33.660	23.636	14.034
1500	12.000	34.490	24.334	15.234
1600	12.000	35.260	24.989	16.434
1700	12.000	35.990	25.617	17.634
1800	12.000	36.670	26.207	18.834
1900	12.000	37.320	26.776	20.034
2000	12.000	37.940	27.323	21.234

*Data for Sm(1) estimated.

Phase changes: 1190 K, α - β transition point of Sm; $\Delta H°$ = 0.744 kcal/mol.
1345 K, melting point of Sm; $\Delta H°$ = 2.060 kcal/mol.
2064 K, boiling point of Sm; $\Delta H°$ = 39.8 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1190 K: $Cp° = 8.200 + 2.970\times10^{-3}T - 1.800\times10^{5}T^{-2}$

$H°- H^{\circ}_{298} = 8.200\times10^{-3}T + 1.485\times10^{-6}T^{2} + 1.800\times10^{2}T^{-1} - 3.181$

1190-1345 K: $Cp° = 11.220$

$H°- H^{\circ}_{298} = 11.220\times10^{-3}T - 3.777$

1345-2000 K: $Cp° = 12.000$

$H°- H^{\circ}_{298} = 12.000\times10^{-3}T - 2.766$

Sources: Entropy at 298 K from Parker (187). All other data from Hultgren (99) who estimated data for Sm(1).

Sm(g)

Samarium (ideal monatomic gas)

[Formation: Sm(c,l) = Sm(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^{\circ}_{298})/T$	$H°-H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	7.255	43.722	43.722	0	49.400	41.323	-30.290
300	7.255	43.767	43.724	.013	49.400	41.271	-30.065
400	7.283	45.857	44.007	.740	49.381	38.562	-21.069
500	7.327	47.486	44.544	1.471	49.266	35.873	-15.680
600	7.368	48.826	45.151	2.205	49.063	33.207	-12.096
700	7.396	49.964	45.758	2.944	48.800	30.590	-9.551
800	7.399	50.952	46.347	3.684	48.507	28.009	-7.652
900	7.373	51.822	46.909	4.422	48.183	25.465	-6.184
1000	7.318	52.597	47.440	5.157	47.847	22.960	-5.018
1100	7.240	53.291	47.941	5.885	47.475	20.480	-4.069
1190	7.153	53.857	48.367	6.534	47.103	18.287	-3.358
1190	7.153	53.857	48.367	6.534	46.359	18.287	-3.358
1200	7.143	53.917	48.413	6.605	46.318	18.062	-3.289
1300	7.036	54.484	48.858	7.314	45.905	15.714	-2.642
1345	6.985	54.723	49.050	7.629	45.715	14.682	-2.386
1345	6.985	54.723	49.050	7.629	43.655	14.682	-2.386
1400	6.922	55.001	49.279	8.011	43.377	13.500	-2.107
1500	6.807	55.475	49.676	8.698	42.864	11.387	-1.659
1600	6.695	55.911	50.053	9.373	42.339	9.297	-1.270
1700	6.589	56.313	50.409	10.037	41.803	7.254	-.933
1800	6.490	56.687	50.748	10.691	41.257	5.226	-.635
1900	6.401	57.036	51.070	11.335	40.701	3.241	-.373
2000	6.323	57.362	51.376	11.972	40.138	1.294	-.141

Phase changes: 1190 K, α - β transition point of Sm; $\Delta H° = 0.744$ kcal/mol.
1345 K, melting point of Sm; $\Delta H° = 2.060$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.895 - 0.670\times10^{-3}T - 0.391\times10^{5}T^{-2}$

$H°-H^{\circ}_{298} = 7.895\times10^{-3}T - 0.335\times10^{-6}T^{2} + 0.391\times10^{2}T^{-1} - 2.455$

Formation equations (kcal/mol):

298.15-1190 K: $\Delta Hf° = 50.125 - 0.305\times10^{-3}T - 1.820\times10^{-6}T^{2} - 140.900T^{-1}$

$\Delta Gf° = 50.125 + 0.305\times10^{-3}T\ln T + 1.820\times10^{-6}T^{2} - 70.450T^{-1} - 31.013\times10^{-3}T$

1190-1345 K: $\Delta Hf° = 50.721 - 3.325\times10^{-3}T - 0.335\times10^{-6}T^{2} + 39.100T^{-1}$

$\Delta Gf° = 50.721 + 3.325\times10^{-3}T\ln T + 0.335\times10^{-6}T^{2} + 19.550T^{-1} - 51.196\times10^{-3}T$

1345-2000 K: $\Delta Hf° = 49.710 - 4.105\times10^{-3}T - 0.335\times10^{-6}T^{2} + 39.100T^{-1}$

$\Delta Gf° = 49.710 + 4.105\times10^{-3}T\ln T + 0.335\times10^{-6}T^{2} + 19.550T^{-1} - 56.064\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). All other data from Feber (58).

Sm_2O_3(cubic)

Disamarium Trioxide, Samarium Sesquioxide

[Formation: $2Sm(c) + 1.5O_2(g) = Sm_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	27.686	34.600	34.600	0	-436.760	-415.243	304.378
300	27.742	34.771	34.601	.051	-436.755	-415.112	302.405
400	30.065	43.099	35.719	2.952	-436.411	-407.948	222.890
500	31.591	49.982	37.904	6.039	-436.112	-400.862	175.214
600	32.720	55.846	40.418	9.257	-435.901	-393.841	143.455
700	33.592	60.958	42.995	12.574	-435.755	-386.834	120.774
800	34.262	65.489	45.529	15.968	-435.624	-379.855	103.770
900	34.759	69.555	47.976	19.421	-435.516	-372.890	90.549
1000	35.097	73.236	50.321	22.915	-435.404	-365.935	79.974
1100	35.284	76.591	52.559	26.435	-435.342	-359.009	71.328
1150	35.322	78.160	53.638	28.200	-435.337	-355.544	67.568

*Entropy at 298 K estimated.

Phase change: 1150 K, cubic to monoclinic transition above 1150 K. Monoclinic form metastable below 1150 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1150 K: $Cp° = 30.831 + 4.834x10^{-3}T - 4.077x10^{5}T^{-2}$

$H°- H°_{298} = 30.831x10^{-3}T + 2.417x10^{-6}T^{2} + 4.077x10^{2}T^{-1} - 10.775$

Formation equations (kcal/mol):

298.15-1150 K: $\Delta Hf° = -437.646 + 3.586x10^{-3}T - 1.308x10^{-6}T^{2} - 20.100T^{-1}$

$\Delta Gf° = -437.646 - 3.586x10^{-3}T\ln T + 1.308x10^{-6}T^{2} - 10.050T^{-1} + 95.292x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Baker (9). Entropy at 298 K estimated using data from Hoekstra (95). High-temperature data based on Pankratz (179).

Sm_2O_3(monoclinic)

Disamarium Trioxide, Samarium Sesquioxide

[Formation: $2Sm(c,l) + 1.5O_2(g) = Sm_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	27.370	36.100	36.100	0	-435.860	-414.790	304.046
300	27.430	36.269	36.100	.051	-435.854	-414.661	302.077
400	29.745	44.505	37.208	2.919	-435.543	-407.643	222.723
500	31.267	51.316	39.368	5.974	-435.277	-400.694	175.141
600	32.411	57.122	41.855	9.160	-435.097	-393.803	143.441
700	33.318	62.189	44.406	12.448	-434.980	-386.922	120.801
800	34.039	66.687	46.914	15.818	-434.874	-380.063	103.827
900	34.592	70.729	49.339	19.251	-434.785	-373.217	90.628
1000	34.981	74.396	51.665	22.731	-434.688	-366.379	80.071
1100	35.204	77.742	53.887	26.241	-434.636	-359.569	71.439
1190*	35.253	80.514	55.797	29.414	-434.650	-353.426	64.908
1190	35.253	80.514	55.797	29.414	-436.138	-353.426	64.908
1195	35.256	80.662	55.900	29.590	-436.137	-353.057	64.569
1195	36.900	80.871	55.900	29.840	-435.887	-353.057	64.569
1200	36.900	81.025	56.005	30.024	-435.879	-352.711	64.237
1300	36.900	83.978	58.044	33.714	-435.717	-345.808	58.135
1345	36.900	85.234	58.933	35.375	-435.649	-342.677	55.681
1345	36.900	85.234	58.933	35.375	-439.769	-342.677	55.681
1400	36.900	86.713	59.996	37.404	-439.773	-338.712	52.875
1500	36.900	89.259	61.863	41.094	-439.788	-331.488	48.297
1600	36.900	91.640	63.650	44.784	-439.814	-324.280	44.294
1700	36.900	93.877	65.363	48.474	-439.847	-317.049	40.759
1800	36.900	95.986	67.006	52.164	-439.889	-309.844	37.620
1900	36.900	97.981	68.584	55.854	-439.940	-302.615	34.808
2000	36.900	99.874	70.102	59.544	-439.998	-295.368	32.276

*Monoclinic form metastable below 1150 K.

Phase Changes: 1190 K, α - β transition point of Sm; $\Delta H°$ = 0.744 kcal/mol.
1195 K, α - β transition point of Sm_2O_3; $\Delta H°$ = 0.250 kcal/mol.
1345 K, melting point of Sm; $\Delta H°$ = 2.060 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1195 K: $Cp° = 30.484 + 4.888\times10^{-3}T - 4.064\times10^{5}T^{-2}$

$H°- H°_{298} = 30.484\times10^{-3}T + 2.444\times10^{-6}T^2 + 4.064\times10^{2}T^{-1} - 10.669$

1195-2000 K: $Cp° = 36.900$

$H°- H°_{298} = 36.900\times10^{-3}T - 14.256$

Formation equations (kcal/mol):

298.15-1190 K: $\Delta Hf° = -436.640 + 3.239\times10^{-3}T - 1.280\times10^{-6}T^2 - 21.400T^{-1}$

$\Delta Gf° = -436.640 - 3.239\times10^{-3}T\ln T + 1.280\times10^{-6}T^2 - 10.700T^{-1} + 91.477\times10^{-3}T$

1190-1195 K: $\Delta Hf° = -435.449 - 2.801\times10^{-3}T + 1.690\times10^{-6}T^2 + 338.600T^{-1}$

$\Delta Gf° = -435.449 + 2.801\times10^{-3}T\ln T - 1.690\times10^{-6}T^2 + 169.300T^{-1} + 51.110\times10^{-3}T$

1195-1345 K: $\Delta Hf° = -439.036 + 3.615\times10^{-3}T - 0.754\times10^{-6}T^2 - 67.800T^{-1}$

$\Delta Gf° = -439.036 - 3.615\times10^{-3}T\ln T + 0.754\times10^{-6}T^2 - 33.900T^{-1} + 96.796\times10^{-3}T$

1345-2000 K: $\Delta Hf° = -441.058 + 2.055\times10^{-3}T - 0.754\times10^{-6}T^2 - 67.800T^{-1}$

$\Delta Gf° = -441.058 - 2.055\times10^{-3}T\ln T + 0.754\times10^{-6}T^2 - 33.900T^{-1} + 87.061\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Baker (9). Low-temperature heat capacities and entropy at 298 K from Justice (110). High-temperature data based on Pankratz (179).

Sn(β,1)

Tin

T, K	cal/mol•K			$H^\circ - H^\circ_{298}$, kcal/mol
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	
298.15	6.450	12.236	12.236	0
300	6.454	12.276	12.236	.012
400	6.891	14.194	12.497	.679
500	7.323	15.778	12.998	1.390
505.12	7.345	15.851	13.024	1.428
505.12	7.100	19.177	13.024	3.108
600	6.875	20.374	14.101	3.764
700	6.817	21.429	15.075	4.448
800	6.800	22.337	15.927	5.128
900	6.800	23.138	16.685	5.808
1000	6.800	23.854	17.366	6.488
1100	6.800	24.502	17.986	7.168
1200	6.800	25.094	18.554	7.848
1300	6.800	25.638	19.078	8.528
1400*	6.800	26.143	19.566	9.208
1500	6.800	26.612	20.020	9.888
1600	6.800	27.050	20.445	10.568
1700	6.800	27.462	20.846	11.248
1800	6.800	27.851	21.224	11.928
1900	6.800	28.219	21.583	12.608
2000	6.800	28.567	21.923	13.288

*Data above 1300 K extrapolated.

Phase changes: 286.2 K α - β transition of Sn; ΔH° = 0.470 kcal/mol.
505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.
2876 K, boiling point of Sn; ΔH° = 70.7 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-505.12 K: $Cp^\circ = 4.968 + 4.684\times10^{-3}T + 0.076\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.968\times10^{-3}T + 2.342\times10^{-6}T^2 - 0.076\times10^{2}T^{-1} - 1.664$

505.12-2000 K: $Cp^\circ = 6.191 + 0.362\times10^{-3}T + 1.854\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.191\times10^{-3}T + 0.181\times10^{-6}T^2 - 1.854\times10^{2}T^{-1} + 0.302$

Source: Data from Hultgren (99) who extrapolated above 1300 K by assuming constant heat capacity.

Sn(g)

Tin (ideal monatomic gas)

[Formation: Sn(c,l) = Sn(g)]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.081	40.244	40.244	0	71.990	63.639	-46.648
300	5.085	40.275	40.245	.009	71.987	63.587	-46.323
400	5.470	41.784	40.446	.535	71.846	60.810	-33.225
500	6.053	43.066	40.846	1.110	71.710	58.066	-25.380
505.12	6.084	43.128	40.869	1.141	71.703	57.925	-25.062
505.12	6.084	43.128	40.869	1.141	70.023	57.925	-25.062
600	6.663	44.224	41.314	1.746	69.972	55.662	-20.275
700	7.184	45.292	41.806	2.440	69.982	53.278	-16.634
800	7.565	46.278	42.306	3.178	70.040	50.887	-13.902
900	7.801	47.183	42.796	3.948	70.130	48.489	-11.775
1000	7.910	48.012	43.278	4.734	70.236	46.078	-10.070
1100	7.919	48.767	43.742	5.527	70.349	43.658	-8.674
1200	7.858	49.454	44.191	6.316	70.458	41.226	-7.508
1300	7.753	50.079	44.620	7.097	70.559	38.786	-6.520
1400	7.623	50.649	45.030	7.866	70.648	36.340	-5.673
1500	7.484	51.170	45.423	8.621	70.723	33.886	-4.937
1600	7.344	51.649	45.798	9.362	70.784	31.426	-4.292
1700	7.211	52.090	46.155	10.090	70.832	28.964	-3.724
1800	7.086	52.498	46.495	10.805	70.867	26.502	-3.218
1900	6.972	52.879	46.822	11.508	70.890	24.036	-2.765
2000	6.869	53.233	47.133	12.200	70.902	21.570	-2.357

Phase change: 505.12 K, melting point of Sn; $\Delta H° = 1.680$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.868 + 0.566\times10^{-3}T - 1.739\times10^{5}T^{-2}$

$H°- H°_{298} = 6.868\times10^{-3}T + 0.283\times10^{-6}T^{2} + 1.739\times10^{2}T^{-1} - 2.656$

Formation equations (kcal/mol):

298.15-505.12 K: $\Delta Hf° = 70.998 + 1.900\times10^{-3}T - 2.059\times10^{-6}T^{2} + 181.500T^{-1}$

$\Delta Gf° = 70.998 - 1.900\times10^{-3}T\ln T + 2.059\times10^{-6}T^{2} - 90.750T^{-1} - 15.489\times10^{-3}T$

505.12-2000 K: $\Delta Hf° = 69.032 + 0.677\times10^{-3}T + 0.102\times10^{-6}T^{2} + 359.300T^{-1}$

$\Delta Gf° = 69.032 - 0.677\times10^{-3}T\ln T - 0.102\times10^{-6}T^{2} + 179.650T^{-1} - 18.468\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (36). All other data from Hilsenrath (94).

SnO(c)

Tin Oxide

[Formation: $Sn(c,l) + 0.5O_2(g) = SnO(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.417	13.665	13.665	0	-68.350	-61.471	45.059
300	11.437	13.736	13.666	.021	-68.347	-61.428	44.750
400	12.220	17.145	14.125	1.208	-68.182	-59.145	32.315
500	12.700	19.926	15.016	2.455	-68.012	-56.906	24.873
505.12	12.718	20.055	15.066	2.520	-68.004	-56.793	24.572
505.12	12.718	20.055	15.066	2.520	-69.684	-56.793	24.572
600	13.061	22.275	16.035	3.744	-69.474	-54.386	19.810
700	13.366	24.312	17.075	5.066	-69.226	-51.890	16.201
800	13.640	26.115	18.095	6.416	-68.954	-49.433	13.504
900	13.898	27.736	19.077	7.793	-68.664	-47.009	11.415
1000	14.144	29.213	20.018	9.195	-68.356	-44.620	9.752

*Data above 298 K estimated.

Phase changes: 505.12 K, melting point of Sn; $\Delta H° = 1.680$ kcal/mol.
1250 K, approximate melting point of SnO; $\Delta H° = 5$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 12.068 + 2.192\times10^{-3}T - 1.160\times10^{5}T^{-2}$

$H°- H°_{298} = 12.068\times10^{-3}T + 1.096\times10^{-6}T^{2} + 1.160\times10^{2}T^{-1} - 4.085$

Formation equations (kcal/mol):

298.15-505.12 K: $\Delta Hf° = -69.595 + 3.485\times10^{-3}T - 1.498\times10^{-6}T^{2} + 101.000T^{-1}$

$\Delta Gf° = -69.595 - 3.485\times10^{-3}T\ln T + 1.498\times10^{-6}T^{2} + 50.500T^{-1} + 46.090\times10^{-3}T$

505.12-1000 K: $\Delta Hf° = -71.560 + 2.262\times10^{-3}T + 0.664\times10^{-6}T^{2} + 278.800T^{-1}$

$\Delta Gf° = -71.560 - 2.262\times10^{-3}T\ln T - 0.664\times10^{-6}T^{2} + 139.400T^{-1} + 43.111\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities and entropy at 298 K from Kostryukov (139). High temperature data estimated. Fusion data from Carbo-Novor (22) who also gives some evidence that SnO(c) is not stable below 1373 K.

$SnO_2(c)$

Tin Dioxide

[Formation: $Sn(c,l) + O_2(g) = SnO_2(c)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.570	12.510	12.510	0	-138.820	-124.291	91.106
300	12.587	12.588	12.511	.023	-138.822	-124.201	90.479
400	14.523	16.477	13.027	1.380	-138.842	-119.319	65.192
500	16.204	19.905	14.067	2.919	-138.745	-114.448	50.025
505.12	16.271	20.070	14.127	3.002	-138.738	-114.201	49.410
505.12	16.271	20.070	14.127	3.002	-140.418	-114.201	49.410
600	17.519	22.981	15.301	4.608	-140.185	-109.291	39.809
700	18.491	25.759	16.600	6.411	-139.844	-104.168	32.522
800	19.182	28.276	17.905	8.297	-139.436	-99.099	27.072
900	19.656	30.564	19.185	10.241	-138.986	-94.082	22.846
1000	19.976	32.653	20.430	12.223	-138.511	-89.120	19.477
1100	20.194	34.568	21.630	14.232	-138.021	-84.205	16.730
1200	20.353	36.332	22.782	16.260	-137.521	-79.333	14.448
1300	20.485	37.966	23.888	18.302	-137.015	-74.504	12.525
1400	20.610	39.489	24.948	20.357	-136.504	-69.714	10.883
1500	20.736	40.915	25.966	22.424	-135.987	-64.962	9.465
1600	20.859	42.257	26.942	24.504	-135.464	-60.245	8.229
1700	20.964	43.525	27.881	26.595	-134.935	-55.560	7.143
1800	21.023	44.725	28.783	28.695	-134.403	-50.905	6.181

Phase change: 505.12 K, melting point of Sn; $\Delta H° = 1.680$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 15.886 + 3.978\times10^{-3}T - 4.002\times10^{5}T^{-2}$

$H°- H°_{298} = 15.886\times10^{-3}T + 1.989\times10^{-6}T^{2} + 4.002\times10^{2}T^{-1} - 6.255$

Formation equations (kcal/mol):

298.15-505.12 K: $\Delta Hf° = -141.060 + 3.688\times10^{-3}T - 0.856\times10^{-6}T^{2} + 362.600T^{-1}$

$\Delta Gf° = -141.060 - 3.688\times10^{-3}T\ln T + 0.856\times10^{-6}T^{2} + 181.300T^{-1} + 74.961\times10^{-3}T$

505.12 1800 K: $\Delta Hf° = -143.025 + 2.465\times10^{-3}T + 1.305\times10^{-6}T^{2} + 540.400T^{-1}$

$\Delta Gf° = -143.025 - 2.465\times10^{-3}T\ln T - 1.305\times10^{-6}T^{2} + 270.200T^{-1} + 71.982\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities and entropy at 298 K from Millar (156). High-temperature data based on Kapustinskii (114).

Sr(c,l,g)

Strontium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15*	6.393	12.500	12.500	0
300	6.400	12.540	12.500	.012
400	6.790	14.434	12.757	.671
500	7.200	15.992	13.252	1.370
600	7.650	17.343	13.823	2.112
700	8.180	18.561	14.414	2.903
800	8.800	19.692	15.003	3.751
828	8.990	19.998	15.167	4.000
828	9.000	20.215	15.167	4.180
900	9.000	20.966	15.602	4.828
1000	9.000	21.915	16.187	5.728
1041	9.000	22.277	16.420	6.097
1041	8.400	24.160	16.420	8.057
1100	8.400	24.622	16.847	8.552
1200	8.400	25.353	17.526	9.392
1300	8.400	26.025	18.154	10.232
1400	8.400	26.648	18.739	11.072
1500	8.400	27.227	19.286	11.912
1600	8.400	27.770	19.800	12.752
1654.1	8.400	28.049	20.064	13.207
1654.1	4.978	47.836	20.064	45.937
1700	4.981	47.972	20.816	46.166
1800	4.991	48.257	22.333	46.664
1900	5.007	48.528	23.705	47.164
2000	5.031	48.785	24.952	47.666

*Data for Sr(c,1) estimated except temperatures of transition and fusion.

Phase changes: 828 K, $\alpha - \gamma$ transition point of Sr; $\Delta H^\circ = 0.180$ kcal/mol.
1041 K, melting point of Sr; $\Delta H^\circ = 1.960$ kcal/mol.
1654.1 K, boiling point of Sr; $\Delta H^\circ = 32.730$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-828 K: $Cp^\circ = 4.594 + 5.064\times10^{-3}T + 0.257\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.594\times10^{-3}T + 2.532\times10^{-6}T^2 - 0.257\times10^{2}T^{-1} - 1.509$

828-1041 K: $Cp^\circ = 9.000$

$H^\circ - H^\circ_{298} = 9.000\times10^{-3}T - 3.272$

1041-1654.1 K: $Cp^\circ = 8.400$

$H^\circ - H^\circ_{298} = 8.400\times10^{-3}T - 0.687$

1654.1-2000 K: $Cp^\circ = 10.273 - 1.950\times10^{-3}T - 56.607\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.273\times10^{-3}T - 0.975\times10^{-6}T^2 + 56.607\times10^{2}T^{-1} + 28.190$

Source: Data from Chase (31) who estimated data for Sr(c,1) except temperatures of transitions and fusion.

Sr(g)

Strontium (ideal monatomic gas)

[Formation: Sr(c,l,g) = Sr(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	39.323	39.323	0	39.200	31.203	-22.872
300	4.968	39.354	39.324	.009	39.197	31.153	-22.695
400	4.968	40.783	39.518	.506	39.035	28.495	-15.569
500	4.968	41.892	39.886	1.003	38.833	25.883	-11.313
600	4.968	42.797	40.297	1.500	38.588	23.316	-8.493
700	4.968	43.563	40.712	1.996	38.293	20.792	-6.491
800	4.968	44.227	41.111	2.493	37.942	18.314	-5.003
828	4.968	44.398	41.219	2.632	37.832	17.629	-4.653
828	4.968	44.398	41.219	2.632	37.652	17.629	-4.653
900	4.968	44.812	41.490	2.990	37.362	15.901	-3.861
1000	4.968	45.335	41.848	3.487	36.959	13.539	-2.959
1041	4.968	45.535	41.989	3.691	36.794	12.583	-2.642
1041	4.968	45.535	41.989	3.691	34.834	12.583	-2.642
1100	4.968	45.809	42.187	3.984	34.632	11.326	-2.250
1200	4.968	46.241	42.508	4.480	34.288	9.222	-1.680
1300	4.968	46.639	42.811	4.977	33.945	7.147	-1.201
1400	4.969	47.007	43.097	5.474	33.602	5.099	-.796
1500	4.971	47.350	43.369	5.971	33.259	3.075	-.448
1600	4.974	47.671	43.629	6.468	32.916	1.074	-.147
1654.1	4.978	47.836	43.763	6.737	32.730	0	0
1654.1	4.978	47.836	43.763	6.737	0	0	0
1700	4.981	47.972	43.874	6.966	0	0	0
1800	4.991	48.257	44.110	7.464	0	0	0
1900	5.007	48.528	44.336	7.964	0	0	0
2000	5.031	48.785	44.552	8.466	0	0	0

Phase changes: 828 K, α - γ transition point of Sr; $\Delta H° = 0.180$ kcal/mol.
1041 K, melting point of Sr; $\Delta H° = 1.960$ kcal/mol.
1654.1 K, boiling point of Sr; $\Delta H° = 32.730$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.959 + 0.010\times10^{-3}T + 0.006\times10^{5}T^{-2}$

$H°- H°_{298} = 4.959\times10^{-3}T + 0.005\times10^{-6}T^{2} - 0.006\times10^{2}T^{-1} - 1.477$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf° = 39.232 + 0.365\times10^{-3}T - 2.527\times10^{-6}T^{2} + 25.100T^{-1}$

$\Delta Gf° = 39.232 - 0.365\times10^{-3}T\ln T + 2.527\times10^{-6}T^{2} + 12.550T^{-1} - 25.744\times10^{-3}T$

828-1041 K: $\Delta Hf° = 40.995 - 4.041\times10^{-3}T + 0.005\times10^{-6}T^{2} - 0.600T^{-1}$

$\Delta Gf° = 40.995 + 4.041\times10^{-3}T\ln T - 0.005\times10^{-6}T^{2} - 0.300T^{-1} - 55.362\times10^{-3}T$

1041-1654.1 K: $\Delta Hf° = 38.410 - 3.441\times10^{-3}T + 0.005\times10^{-6}T^{2} - 0.600T^{-1}$

$\Delta Gf° = 38.410 + 3.441\times10^{-3}T\ln T - 0.005\times10^{-6}T^{2} - 0.300T^{-1} - 48.711\times10^{-3}T$

1654.1-2000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Source: Data from Chase (31).

SrO(c)

Strontium Oxide

[Formation: $Sr(c,l,g) + 0.5O_2(g) = SrO(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.760	13.000	13.000	0	-141.140	-133.984	98.211
300	10.777	13.067	13.000	.020	-141.138	-133.939	97.573
400	11.551	16.285	13.435	1.140	-141.033	-131.555	71.877
500	12.061	18.920	14.276	2.322	-140.915	-129.199	56.472
600	12.449	21.155	15.240	3.549	-140.808	-126.866	46.210
700	12.760	23.098	16.227	4.810	-140.727	-124.549	38.885
800	13.015	24.819	17.195	6.099	-140.684	-122.242	33.395
828	13.074	25.268	17.461	6.464	-140.681	-121.597	32.095
828	13.074	25.268	17.461	6.464	-140.861	-121.597	32.095
900	13.226	26.365	18.131	7.411	-140.857	-119.922	29.121
1000	13.403	27.768	19.025	8.743	-140.838	-117.596	25.700
1041	13.465	28.308	19.380	9.294	-140.827	-116.643	24.488
1041	13.465	28.308	19.380	9.294	-142.787	-116.643	24.488
1100	13.554	29.052	19.878	10.091	-142.733	-115.162	22.880
1200	13.685	30.238	20.694	11.453	-142.635	-112.661	20.518
1300	13.801	31.338	21.471	12.827	-142.530	-110.168	18.521
1400	13.910	32.364	22.212	14.213	-142.415	-107.681	16.810
1500	14.017	33.328	22.922	15.609	-142.294	-105.206	15.328
1600	14.126	34.236	23.601	17.016	-142.166	-102.736	14.033
1654.1	14.189	34.707	23.956	17.782	-142.093	-101.405	13.398
1654.1	14.189	34.707	23.956	17.782	-174.823	-101.405	13.398
1700	14.243	35.096	24.252	18.435	-174.602	-99.372	12.775
1800	14.374	35.913	24.876	19.866	-174.113	-94.958	11.529

Phase changes: 828 K, α - γ transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 11.900 + 1.548\times10^{-3}T - 1.424\times10^{5}T^{-2}$

$H°- H°_{298} = 11.900\times10^{-3}T + 0.774\times10^{-6}T^{2} + 1.424\times10^{2}T^{-1} - 4.094$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf° = -142.550 + 3.691\times10^{-3}T - 2.010\times10^{-6}T^{2} + 145.500T^{-1}$

$\Delta Gf° = -142.550 - 3.691\times10^{-3}T\ln T + 2.010\times10^{-6}T^{2} + 72.750T^{-1} + 48.343\times10^{-3}T$

828-1041 K: $\Delta Hf° = -140.787 - 0.715\times10^{-3}T + 0.523\times10^{-6}T^{2} + 119.800T^{-1}$

$\Delta Gf° = -140.787 + 0.715\times10^{-3}T\ln T - 0.523\times10^{-6}T^{2} + 59.900T^{-1} + 18.725\times10^{-3}T$

1041-1654.1 K: $\Delta Hf° = -143.371 - 0.115\times10^{-3}T + 0.523\times10^{-6}T^{2} + 119.800T^{-1}$

$\Delta Gf° = -143.371 + 0.115\times10^{-3}T\ln T - 0.523\times10^{-6}T^{2} + 59.900T^{-1} + 25.377\times10^{-3}T$

1654.1-1800 K: $\Delta Hf° = -172.248 - 1.988\times10^{-3}T + 1.497\times10^{-6}T^{2} - 5540.900T^{-1}$

$\Delta Gf° = -172.248 + 1.988\times10^{-3}T\ln T - 1.497\times10^{-6}T^{2} - 2770.450T^{-1} + 31.601\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Brink (20). Entropy at 298 K from Parker (180). Low-temperature heat capacities from Anderson (4). High-temperature data based on Lander (141).

SrO(g)

Strontium Oxide (ideal gas)

[Formation: $Sr(c,l,g) + 0.5O_2(g) = SrO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.909	54.958	54.958	0	-3.200	-8.553	6.270
300	7.918	55.007	54.957	.015	-3.204	-8.586	6.255
400	8.276	57.338	55.273	.826	-3.407	-10.350	5.655
500	8.498	59.211	55.881	1.665	-3.632	-12.061	5.272
600	8.641	60.773	56.568	2.523	-3.894	-13.722	4.998
700	8.738	62.113	57.267	3.392	-4.205	-15.337	4.788
800	8.808	63.285	57.949	4.269	-4.575	-16.905	4.618
828	8.824	63.588	58.134	4.516	-4.690	-17.334	4.575
828	8.824	63.588	58.134	4.516	-4.870	-17.335	4.575
900	8.864	64.326	58.600	5.153	-5.175	-18.405	4.469
1000	8.917	65.262	59.220	6.042	-5.599	-19.851	4.338
1041	8.942	65.621	59.465	6.408	-5.773	-20.431	4.289
1041	8.942	65.621	59.465	6.408	-7.733	-20.431	4.289
1100	8.977	66.115	59.809	6.937	-7.948	-21.145	4.201
1200	9.057	66.899	60.367	7.838	-8.311	-22.329	4.067
1300	9.168	67.628	60.898	8.749	-8.668	-23.483	3.948
1400	9.322	68.313	61.404	9.673	-9.015	-24.609	3.842
1500	9.527	68.963	61.886	10.615	-9.349	-25.713	3.746
1600	9.789	69.586	62.348	11.581	-9.661	-26.791	3.659
1654.1	9.962	69.913	62.589	12.114	-9.821	-27.368	3.616
1654.1	9.962	69.913	62.589	12.114	-42.551	-27.368	3.616
1700	10.108	70.188	62.791	12.575	-42.522	-26.948	3.464
1800	10.482	70.777	63.219	13.604	-42.435	-26.035	3.161
1900	10.905	71.354	63.631	14.673	-42.313	-25.125	2.890
2000	11.364	71.925	64.032	15.786	-42.152	-24.226	2.647

Phase changes: 828 K, α - γ transition point of Sr; $\Delta H°$ = 0.180 kcal/mol.
1041 K, melting point of Sr; $\Delta H°$ = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; $\Delta H°$ = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.812 + 1.266\times10^{-3}T - 0.249\times10^{5}T^{-2}$

$H°- H°_{298} = 7.812\times10^{-3}T + 0.633\times10^{-6}T^2 + 0.249\times10^{2}T^{-1} - 2.469$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf° = -2.984 - 0.397\times10^{-3}T - 2.151\times10^{-6}T^2 + 28.000T^{-1}$

$\Delta Gf° = -2.984 + 0.397\times10^{-3}T\ln T + 2.151\times10^{-6}T^2 + 14.000T^{-1} - 21.739\times10^{-3}T$

828-1041 K: $\Delta Hf° = -1.221 - 4.803\times10^{-3}T + 0.382\times10^{-6}T^2 + 2.300T^{-1}$

$\Delta Gf° = -1.221 + 4.803\times10^{-3}T\ln T - 0.382\times10^{-6}T^2 + 1.150T^{-1} - 51.358\times10^{-3}T$

1041-1654.1 K: $\Delta Hf° = -3.806 - 4.203\times10^{-3}T + 0.382\times10^{-6}T^2 + 2.300T^{-1}$

$\Delta Gf° = -3.806 + 4.203\times10^{-3}T\ln T - 0.382\times10^{-6}T^2 + 1.150T^{-1} - 44.706\times10^{-3}T$

1654.1-2000 K: $\Delta Hf° = -32.683 - 6.076\times10^{-3}T + 1.357\times10^{-6}T^2 - 5658.400T^{-1}$

$\Delta Gf° = -32.683 + 6.076\times10^{-3}T\ln T - 1.357\times10^{-6}T^2 - 2829.200T^{-1} - 38.482\times10^{-3}T$

Source: Data from Chase (33).

Ta(c,l)

Tantalum

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.060	9.920	9.920	0
300	6.060	9.960	9.923	.011
400	6.220	11.728	10.160	.627
500	6.280	13.123	10.619	1.252
600	6.330	14.272	11.135	1.882
700	6.390	15.252	11.655	2.518
800	6.450	16.109	12.159	3.160
900	6.510	16.872	12.641	3.808
1000	6.570	17.561	13.099	4.462
1100	6.630	18.190	13.534	5.122
1200	6.690	18.770	13.947	5.788
1300	6.770	19.309	14.339	6.461
1400	6.850	19.813	14.712	7.142
1500	6.940	20.289	15.068	7.832
1600	7.040	20.740	15.408	8.531
1700	7.120	21.169	15.734	9.239
1800	7.230	21.579	16.048	9.956
1900	7.340	21.973	16.350	10.684
2000	7.450	22.351	16.639	11.423
2100	7.580	22.718	16.921	12.174
2200	7.710	23.073	17.192	12.938
2300	7.850	23.419	17.456	13.716
2400	8.000	23.756	17.711	14.508
2500	8.170	24.086	17.960	15.316
2600	8.360	24.410	18.201	16.143
2700	8.580	24.730	18.437	16.990
2800	8.830	25.046	18.667	17.860
2900	9.130	25.361	18.893	18.756
3000	9.470	25.676	19.114	19.685
3100	9.910	25.993	19.331	20.652
3200	10.650	26.318	19.544	21.678
3258	11.230	26.515	19.669	22.305
3258*	10.000	28.835	19.669	29.865
3300	10.000	28.964	19.787	30.285
3400	10.000	29.262	20.061	31.285
3500	10.000	29.552	20.328	32.285

*Data for Ta(l) estimated.

Phase change: 3258 K, melting point of Ta; ΔH° = 7.560 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3258 K: $Cp^\circ = 5.056 + 1.364\times10^{-3}T + 0.532\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.056\times10^{-3}T + 0.682\times10^{-6}T^2 - 0.532\times10^{2}T^{-1} - 1.390$

3258-3500 K: $Cp^\circ = 10.000$

$H^\circ - H^\circ_{298} = 10.000\times10^{-3}T - 2.715$

Sources: Temperature of fusion from Cezairliyan (23). All other data from Hultgren (99) who estimated data for Ta(l).

Ta(g)

Tantalum (ideal monatomic gas)

[Formation: Ta(c) = Ta(g)]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.985	44.242	44.242	0	186.900	176.667	-129.499
300	4.986	44.272	44.242	.009	186.898	176.604	-128.655
400	5.081	45.717	44.437	.512	186.785	173.189	-94.625
500	5.278	46.871	44.813	1.029	186.677	169.803	-74.220
600	5.541	47.855	45.240	1.569	186.587	166.437	-60.624
700	5.827	48.731	45.677	2.138	186.520	163.085	-50.917
800	6.109	49.528	46.109	2.735	186.475	159.740	-43.638
900	6.376	50.263	46.531	3.359	186.451	156.399	-37.978
1000	6.621	50.947	46.938	4.009	186.447	153.061	-33.451
1100	6.843	51.589	47.332	4.683	186.461	149.722	-29.747
1200	7.043	52.193	47.712	5.377	186.489	146.381	-26.659
1300	7.221	52.764	48.079	6.090	186.529	143.037	-24.046
1400	7.377	53.305	48.434	6.820	186.578	139.689	-21.806
1500	7.514	53.819	48.776	7.565	186.633	136.338	-19.864
1600	7.633	54.308	49.106	8.323	186.692	132.983	-18.164
1700	7.738	54.774	49.426	9.091	186.752	129.623	-16.664
1800	7.831	55.219	49.736	9.870	186.814	126.262	-15.330
1900	7.915	55.644	50.035	10.657	186.873	122.898	-14.136
2000	7.992	56.052	50.325	11.453	186.930	119.528	-13.061

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.349 + 2.094\times10^{-3}T + 0.010\times10^{5}T^{-2}$

$H°- H°_{298} = 4.349\times10^{-3}T + 1.047\times10^{-6}T^{2} - 0.010\times10^{2}T^{-1} - 1.386$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 186.903 - 0.707\times10^{-3}T + 0.365\times10^{-6}T^{2} + 52.200T^{-1}$

$\Delta Gf° = 186.903 + 0.707\times10^{-3}T\ln T - 0.365\times10^{-6}T^{2} + 26.100T^{-1} - 38.546\times10^{-3}T$

Source: Data from Chase (33).

TaO(g)

Tantalum Oxide (ideal gas)

[Formation: $Ta(c) + 0.5O_2(g) = TaO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.314	57.601	57.601	0	46.000	39.089	-28.653
300	7.320	57.646	57.601	.014	45.996	39.048	-28.446
400	7.681	59.802	57.892	.764	45.776	36.764	-20.087
500	7.988	61.550	58.454	1.548	45.569	34.536	-15.095
600	8.237	63.029	59.097	2.359	45.373	32.347	-11.782
700	8.447	64.315	59.752	3.194	45.182	30.192	-9.426
800	8.637	65.456	60.396	4.048	44.995	28.062	-7.666
900	8.813	66.483	61.015	4.921	44.814	25.957	-6.303
1000	8.978	67.421	61.611	5.810	44.635	23.870	-5.217
1100	9.130	68.283	62.178	6.716	44.461	21.804	-4.332
1200	9.268	69.084	62.721	7.636	44.292	19.752	-3.597
1300	9.392	69.831	63.239	8.569	44.124	17.713	-2.978
1400	9.503	70.531	63.735	9.514	43.956	15.687	-2.449
1500	9.601	71.190	64.211	10.469	43.786	13.674	-1.992
1600	9.691	71.813	64.667	11.434	43.613	11.671	-1.594
1700	9.775	72.403	65.105	12.407	43.437	9.680	-1.244
1800	9.856	72.964	65.526	13.389	43.258	7.701	-.935
1900	9.936	73.499	65.931	14.379	43.073	5.731	-.659
2000	10.018	74.010	66.322	15.376	42.882	3.770	-.412

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.677 + 1.288\times10^{-3}T - 0.664\times10^{5}T^{-2}$

$H°- H°_{298} = 7.677\times10^{-3}T + 0.644\times10^{-6}T^{2} + 0.664\times10^{2}T^{-1} - 2.569$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 45.997 - 0.994\times10^{-3}T - 0.289\times10^{-6}T^{2} + 97.000T^{-1}$

$\Delta Gf° = 45.997 + 0.994\times10^{-3}T\ln T + 0.289\times10^{-6}T^{2} + 48.500T^{-1} - 29.463\times10^{-3}T$

Source: Data from Chase (33).

$TaO_2(g)$

Tantalum Dioxide (ideal gas)

[Formation: $Ta(c) + O_2(g) = TaO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	10.516	66.957	66.957	0	-48.000	-50.395	36.940
300	10.534	67.023	66.960	.019	-48.005	-50.409	36.723
400	11.407	70.178	67.383	1.118	-48.232	-51.176	27.961
500	12.047	72.796	68.210	2.293	-48.413	-51.889	22.680
600	12.495	75.035	69.167	3.521	-48.570	-52.570	19.148
700	12.810	76.986	70.147	4.787	-48.718	-53.225	16.617
800	13.035	78.712	71.112	6.080	-48.865	-53.859	14.714
900	13.200	80.257	72.044	7.392	-49.015	-54.474	13.228
1000	13.324	81.654	72.935	8.719	-49.169	-55.072	12.036
1100	13.418	82.929	73.787	10.056	-49.331	-55.655	11.057
1200	13.492	84.100	74.598	11.402	-49.499	-56.221	10.239
1300	13.552	85.182	75.371	12.754	-49.676	-56.774	9.544
1400	13.600	86.188	76.108	14.112	-49.863	-57.314	8.947
1500	13.641	87.128	76.812	15.474	-50.061	-57.840	8.427
1600	13.675	88.009	77.484	16.840	-50.271	-58.351	7.970
1700	13.706	88.839	78.128	18.209	-50.492	-58.849	7.565
1800	13.735	89.624	78.746	19.581	-50.725	-59.334	7.204
1900	13.762	90.367	79.338	20.956	-50.972	-59.805	6.879
2000	13.789	91.074	79.908	22.333	-51.233	-60.267	6.586

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 12.523 + 0.848\times10^{-3}T - 2.009\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 12.523\times10^{-3}T + 0.424\times10^{-6}T^2 + 2.009\times10^{2}T^{-1} - 4.445$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -48.704 + 0.237\times10^{-3}T - 0.761\times10^{-6}T^2 + 208.900T^{-1}$

$\Delta Gf^\circ = -48.704 - 0.237\times10^{-3}T\ln T + 0.761\times10^{-6}T^2 + 104.450T^{-1} - 5.723\times10^{-3}T$

Source: Data from Chase (33).

$Ta_2O_5(\beta)$

Ditantalum Pentoxide

[Formation: $2Ta(c) + 2.5O_2(g) = Ta_2O_5(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	32.300	34.200	34.200	0	-489.000	-456.754	334.806
300	32.383	34.400	34.200	.060	-488.995	-456.552	332.593
400	35.484	44.207	35.517	3.476	-488.585	-445.796	243.568
500	37.562	52.355	38.093	7.131	-488.008	-435.161	190.206
600	39.318	59.364	41.067	10.978	-487.309	-424.655	154.678
700	40.741	65.536	44.130	14.984	-486.520	-414.274	129.340
800	41.840	71.051	47.157	19.115	-485.668	-404.014	110.370
900	42.670	76.029	50.092	23.343	-484.771	-393.859	95.641
1000	43.310	80.559	52.916	27.643	-483.846	-383.808	83.880
1100	43.842	84.713	55.621	32.001	-482.905	-373.849	74.276
1200	44.340	88.549	58.207	36.410	-481.948	-363.975	66.288
1300	44.867	92.118	60.680	40.870	-480.975	-354.182	59.543
1400	45.464	95.465	63.046	45.386	-479.981	-344.470	53.773
1500	46.155	98.624	65.313	49.966	-478.956	-334.826	48.783
1600	46.939	101.628	67.491	54.620	-477.892	-325.253	44.427
1700	47.796	104.499	69.584	59.356	-476.777	-315.746	40.591
1800	48.679	107.256	71.600	64.180	-475.607	-306.304	37.190
1900	49.519	109.911	73.547	69.091	-474.387	-296.932	34.154
2000	50.223	112.469	75.430	74.079	-473.124	-287.628	31.430

Phase change: 1633 K, β - α transition point of Ta_2O_5. Transition sluggish, no evidence for it in high-temperature data.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 36.953 + 6.554\times10^{-3}T - 5.873\times10^{5}T^{-2}$

$H°- H°_{298} = 36.953\times10^{-3}T + 3.277\times10^{-6}T^{2} + 5.873\times10^{2}T^{-1} - 13.279$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -493.620 + 8.766\times10^{-3}T + 0.656\times10^{-6}T^{2} + 580.700T^{-1}$

$\Delta Gf° = -493.620 - 8.766\times10^{-3}T\ln T - 0.656\times10^{-6}T^{2} + 290.350T^{-1} + 170.521\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (236). Low-temperature heat capacities and entropy at 298 K from Kelley (116). High-temperature data based on Orr (171). Transition data from Reisman (187).

Tb(c,1)

Terbium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.910	17.520	17.520	0
300	6.910	17.560	17.520	.013
400	6.820	19.530	17.785	.698
500	6.760	21.040	18.284	1.378
600	7.160	22.310	18.853	2.074
700	7.510	23.440	19.430	2.807
800	7.840	24.470	20.002	3.574
900	8.200	25.410	20.549	4.375
1000	8.580	26.290	21.075	5.215
1100	8.960	27.130	21.594	6.090
1200	9.370	27.920	22.083	7.004
1300	9.830	28.690	22.565	7.963
1400	10.330	29.440	23.033	8.970
1500	10.850	30.170	23.485	10.028
1560	11.180	30.600	23.746	10.692
1560	6.640	31.370	23.746	11.892
1600	6.640	31.540	23.942	12.157
1630	6.640	31.660	24.078	12.357
1630	11.110	33.240	24.078	14.937
1700	11.110	33.710	24.465	15.717
1800	11.110	34.340	24.992	16.827
1900	11.110	34.940	25.499	17.938
2000	11.110	35.510	25.985	19.049

Phase changes: 1560 K, α - β transition of Tb; ΔH° = 1.200 kcal/mol.
1630 K, melting point of Tb; ΔH° = 2.580 kcal/mol.
3496 K, boiling point of Tb; ΔH° = 79.1 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1560 K: $Cp^\circ = 4.284 + 4.228\times10^{-3}T + 1.214\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.284\times10^{-3}T + 2.114\times10^{-6}T^2 - 1.214\times10^{2}T^{-1} - 1.058$

1560-1630 K: $Cp^\circ = 6.641$

$H^\circ - H^\circ_{298} = 6.641\times10^{-3}T + 1.532$

1630-2000 K: $Cp^\circ = 11.110$

$H^\circ - H^\circ_{298} = 11.110\times10^{-3}T - 3.172$

Source: Data from Hultgren (99).

Tb(g)

Terbium (ideal monatomic gas)

[Formation: Tb(c,1) = Tb(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.895	48.552	48.552	0	92.900	83.648	-61.315
300	5.892	48.588	48.552	.011	92.898	83.590	-60.894
400	5.790	50.267	48.782	.594	92.796	80.501	-43.983
500	5.758	51.554	49.212	1.171	92.693	77.436	-33.847
600	5.781	52.606	49.693	1.748	92.574	74.396	-27.099
700	5.845	53.501	50.174	2.329	92.422	71.379	-22.285
800	5.936	54.287	50.639	2.918	92.244	68.390	-18.683
900	6.046	54.993	51.085	3.517	92.042	65.417	-15.885
1000	6.164	55.636	51.509	4.127	91.812	62.466	-13.652
1100	6.287	56.229	51.911	4.750	91.560	59.551	-11.832
1200	6.408	56.781	52.294	5.384	91.280	56.647	-10.317
1300	6.525	57.299	52.660	6.031	90.968	53.776	-9.041
1400	6.637	57.786	53.008	6.689	90.619	50.935	-7.951
1500	6.740	58.248	53.343	7.358	90.230	48.113	-7.010
1560	6.797	58.513	53.536	7.764	89.972	46.426	-6.504
1560	6.797	58.513	53.536	7.764	88.772	46.426	-6.504
1600	6.835	58.686	53.663	8.037	88.780	45.346	-6.194
1630	6.860	58.813	53.757	8.242	88.785	44.524	-5.970
1630	6.860	58.813	53.757	8.242	86.205	44.524	-5.970
1700	6.920	59.103	53.971	8.725	85.908	42.740	-5.495
1800	6.997	59.501	54.267	9.421	85.494	40.204	-4.881
1900	7.064	59.881	54.553	10.124	85.086	37.698	-4.336
2000	7.123	60.244	54.827	10.833	84.684	35.216	-3.848

Phase changes: 1560 K, α - β transition point of Tb; $\Delta H° = 1.200$ kcal/mol.
1630 K, melting point of Tb; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.975 + 1.142\times10^{-3}T + 0.515\times10^{5}T^{-2}$

$H°- H°_{298} = 4.975\times10^{-3}T + 0.571\times10^{-6}T^{2} - 0.515\times10^{2}T^{-1} - 1.361$

Formation equations (kcal/mol):

298.15-1560 K: $\Delta Hf° = 92.597 + 0.691\times10^{-3}T - 1.543\times10^{-6}T^{2} + 69.900T^{-1}$

$\Delta Gf° = 92.597 - 0.691\times10^{-3}T\ln T + 1.543\times10^{-6}T^{2} + 34.950T^{-1} - 26.931\times10^{-3}T$

1560-1630 K: $\Delta Hf° = 90.007 - 1.666\times10^{-3}T + 0.571\times10^{-6}T^{2} - 51.500T^{-1}$

$\Delta Gf° = 90.007 + 1.666\times10^{-3}T\ln T - 0.571\times10^{-6}T^{2} - 25.750T^{-1} - 39.278\times10^{-3}T$

1630-2000 K: $\Delta Hf° = 94.711 - 6.135\times10^{-3}T + 0.571\times10^{-6}T^{2} - 51.500T^{-1}$

$\Delta Gf° = 94.711 + 6.135\times10^{-3}T\ln T - 0.571\times10^{-6}T^{2} - 25.750T^{-1} - 75.218\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). All other data from Feber (59).

$TbO_{1.719}(c)$

Terbium Oxide

[Formation: $Tb(c) + 0.8595O_2(g) = TbO_{1.719}(c)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	14.100	19.300	19.300	0	-227.800	-215.773	158.164
300	14.128	19.387	19.300	.026	-227.798	-215.699	157.135
400	15.281	23.629	19.872	1.503	-227.616	-211.691	115.661
500	16.026	27.123	20.983	3.070	-227.358	-207.742	90.803
600	16.644	30.100	22.260	4.704	-227.069	-203.845	74.249
700	17.221	32.709	23.569	6.398	-226.776	-199.996	62.441
800	17.793	35.046	24.861	8.148	-226.479	-196.187	53.595
900	18.377	37.175	26.112	9.957	-226.171	-192.420	46.725
1000	18.982	39.143	27.319	11.824	-225.855	-188.693	41.238

*Entropy and heat capacity at 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 14.238 + 4.700\times10^{-3}T - 1.368\times10^{5}T^{-2}$

$H°- H°_{298} = 14.238\times10^{-3}T + 2.350\times10^{-6}T^{2} + 1.368\times10^{2}T^{-1} - 4.913$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf° = -229.633 + 3.740\times10^{-3}T - 0.196\times10^{-6}T^{2} + 219.351T^{-1}$

$\Delta Gf° = -229.633 - 3.740\times10^{-3}T\ln T + 0.196\times10^{-6}T^{2} + 109.675T^{-1} + 66.504\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Fitzgibbon (61). Entropy at 298 K estimated by Westrum (246). Heat capacity at 298 K estimated. High-temperature data based on Pankratz (174).

$TbO_{1.812}(c)$

Terbium Oxide

[Formation: $Tb(c) + 0.906O_2(g) = TbO_{1.812}(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.900	19.400	19.400	0	-229.900	-217.223	159.227
300	13.940	19.486	19.399	.026	-229.899	-217.145	158.188
400	15.540	23.743	19.971	1.509	-229.744	-212.914	116.329
500	16.483	27.319	21.091	3.114	-229.481	-208.738	91.238
600	17.138	30.386	22.393	4.796	-229.179	-204.618	74.531
700	17.619	33.065	23.729	6.535	-228.878	-200.547	62.613
800	17.976	35.443	25.048	8.316	-228.587	-196.516	53.685
900	18.231	37.576	26.324	10.127	-228.315	-192.526	46.751

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp° = 16.033 + 3.044\times10^{-3}T - 2.702\times10^{5}T^{-2}$

$H°- H°_{298} = 16.033\times10^{-3}T + 1.522\times10^{-6}T^{2} + 2.702\times10^{2}T^{-1} - 5.822$

Formation equations (kcal/mol):

298.15-900 K: $\Delta Hf° = -232.533 + 5.199\times10^{-3}T - 1.048\times10^{-6}T^{2} + 350.649T^{-1}$

$\Delta Gf° = -232.533 - 5.199\times10^{-3}T\ln T + 1.048\times10^{-6}T^{2} + 175.324T^{-1} + 78.684\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Fitzgibbon (61). Entropy at 298 K estimated by Westrum (246). Heat capacity at 298 K estimated. High-temperature data based on Pankratz (174).

$Tb_2O_3(c)$

Diterbium Trioxide, Terbium Sesquioxide

[Formation: $2Tb(c,l) + 1.5O_2(g) = Tb_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	27.500	37.500	37.500	0	-445.800	-424.617	311.249
300	27.559	37.670	37.500	.051	-445.794	-424.487	309.235
400	29.669	45.934	38.614	2.928	-445.352	-417.448	228.080
500	30.712	52.677	40.773	5.952	-444.785	-410.543	179.446
600	31.412	58.341	43.241	9.060	-444.201	-403.747	147.063
700	31.998	63.228	45.755	12.231	-443.664	-397.046	123.962
800	32.557	67.537	48.215	15.458	-443.167	-390.413	106.655
900	33.127	71.404	50.580	18.742	-442.706	-383.851	93.211
1000	33.720	74.925	52.840	22.085	-442.284	-377.344	82.467
1100	34.339	78.168	54.998	25.487	-441.891	-370.856	73.681
1200	34.980	81.183	57.056	28.953	-441.524	-364.426	66.370
1300	35.639	84.009	59.021	32.484	-441.195	-358.008	60.186
1400	36.305	86.674	60.902	36.081	-440.909	-351.609	54.888
1500	36.971	89.202	62.705	39.745	-440.665	-345.239	50.301
1560	37.363	90.660	63.753	41.975	-440.552	-341.435	47.833
1560	37.363	90.660	63.753	41.975	-442.952	-341.435	47.833
1600	37.625	91.609	64.437	43.475	-442.509	-338.830	46.281
1630	37.815	92.310	64.944	44.607	-442.174	-336.906	45.172
1630	37.815	92.310	64.944	44.607	-447.334	-336.906	45.172
1700	38.257	93.909	66.104	47.269	-447.158	-332.167	42.702
1800	38.856	96.113	67.710	51.125	-446.854	-325.426	39.512

*Entropy and heat capacity at 298 K estimated.

Phase changes: 1560 K, α - β transition point of Tb; $\Delta H°$ = 1.200 kcal/mol.
1630 K, melting point of Tb; $\Delta H°$ = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 29.306 + 4.952\times10^{-3}T - 2.918\times10^{5}T^{-2}$

$H°- H°_{298} = 29.306\times10^{-3}T + 2.476\times10^{-6}T^{2} + 2.918\times10^{2}T^{-1} - 9.936$

Formation equations (kcal/mol):

298.15-1560 K: $\Delta Hf° = -450.092 + 9.893\times10^{-3}T - 2.506\times10^{-6}T^{2} + 466.800T^{-1}$

$\Delta Gf° = -450.092 - 9.893\times10^{-3}T\ln T + 2.506\times10^{-6}T^{2} + 233.400T^{-1} + 138.438\times10^{-3}T$

1560-1630 K: $\Delta Hf° = -455.272 + 5.179\times10^{-3}T + 1.722\times10^{-6}T^{2} + 224.000T^{-1}$

$\Delta Gf° = -455.272 - 5.179\times10^{-3}T\ln T - 1.722\times10^{-6}T^{2} + 112.000T^{-1} + 113.744\times10^{-3}T$

1630-1800 K: $\Delta Hf° = -445.863 - 3.759\times10^{-3}T + 1.722\times10^{-6}T^{2} + 224.000T^{-1}$

$\Delta Gf° = -445.863 + 3.759\times10^{-3}T\ln T - 1.722\times10^{-6}T^{2} + 112.000T^{-1} + 41.863\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). Entropy at 298 K estimated by Westrum (246). Heat capacity at 298 K estimated. High-temperature data based on Pankratz (174).

Te(c,l)

Tellurium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.140	11.880	11.880	0
300	6.150	11.920	11.883	.011
400	6.680	13.760	12.128	.653
500	7.210	15.310	12.616	1.347
600	7.730	16.670	13.180	2.094
700	8.260	17.900	13.766	2.894
722.65	8.380	18.170	13.899	3.085
722.65	9.000	23.950	13.899	7.265
800	9.000	24.860	14.910	7.960
900	9.000	25.920	16.076	8.860
1000	9.000	26.870	17.110	9.760
1100*	9.000	27.720	18.029	10.660
1200	9.000	28.510	18.877	11.560
1262	9.000	28.960	19.358	12.118

*Data extrapolated 1100 - 1262 K.

Phase changes: 722.65 K, melting point of Te; ΔH° = 4.180 kcal/mol.
1262 K, boiling point of Te to equilibrium mixture, which is predominately $Te_2(g)$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-722.65 K: $Cp^\circ = 4.515 + 5.374\times10^{-3}T + 0.020\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.515\times10^{-3}T + 2.687\times10^{-6}T^2 - 0.020\times10^{2}T^{-1} - 1.578$

722.65-1262 K: $Cp^\circ = 9.000$

$H^\circ - H^\circ_{298} = 9.000\times10^{-3}T + 0.761$

Sources: Entropy at 298 K from Wagman (236). All other data from Hultgren (99) who extrapolated 1100 - 1262 K by assuming constant heat capacity.

Te(g)

Tellurium (ideal monatomic gas)

[Reaction: $0.5Te_2(g) = Te(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH°	ΔG°	
298.15	4.970	43.640	43.640	0	31.435	27.647	-20.266
300	4.970	43.670	43.640	.009	31.436	27.623	-20.123
400	4.930	45.100	43.840	.504	31.491	26.341	-14.392
500	4.930	46.200	44.206	.997	31.536	25.049	-10.949
600	4.950	47.100	44.615	1.491	31.574	23.750	-8.651
700	4.980	47.860	45.020	1.988	31.606	22.447	-7.008
800	5.020	48.530	45.420	2.488	31.633	21.133	-5.773
900	5.060	49.120	45.796	2.992	31.657	19.822	-4.813
1000	5.100	49.660	46.160	3.500	31.676	18.501	-4.043
1100	5.140	50.150	46.504	4.011	31.690	17.181	-3.414
1200	5.180	50.600	46.827	4.527	31.701	15.862	-2.889
1300	5.220	51.010	47.127	5.048	31.710	14.550	-2.446
1400	5.270	51.400	47.420	5.572	31.713	13.226	-2.065
1500	5.310	51.770	47.703	6.101	31.720	11.897	-1.733
1600	5.350	52.110	47.964	6.634	31.731	10.579	-1.445
1700	5.390	52.430	48.212	7.171	31.747	9.273	-1.192
1800	5.440	52.740	48.456	7.712	31.768	7.945	-.965
1900	5.480	53.040	48.694	8.258	31.797	6.612	-.761
2000	5.520	53.320	48.916	8.809	31.833	5.293	-.578

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 4.647 + 0.434\times10^{-3}T + 0.172\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.647\times10^{-3}T + 0.217\times10^{-6}T^2 - 0.172\times10^{2}T^{-1} - 1.347$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = 31.437 + 0.347\times10^{-3}T - 0.079\times10^{-6}T^2 - 29.300T^{-1}$

$\Delta G^\circ = 31.437 - 0.347\times10^{-3}T\ln T + 0.079\times10^{-6}T^2 - 14.650T^{-1} - 10.590\times10^{-3}T$

Source: Data from Mills (158).

$Te_2(g)$

Tellurium (ideal diatomic gas)

[Formation: $2Te(c,l) = Te_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	8.680	61.870	61.870	0	38.330	26.968	-19.767
300	8.680	61.920	61.870	.016	38.324	26.900	-19.596
400	8.870	64.450	62.212	.895	37.919	23.147	-12.647
500	9.050	66.450	62.868	1.791	37.427	19.512	-8.529
600	9.210	68.120	63.613	2.704	36.846	15.978	-5.820
700	9.370	69.550	64.360	3.633	36.175	12.550	-3.918
722.65	9.409	69.849	64.527	3.846	36.006	11.787	-3.565
722.65	9.409	69.849	64.527	3.846	27.646	11.787	-3.565
800	9.540	70.810	65.086	4.579	26.989	10.117	-2.764
900	9.700	71.940	65.784	5.540	26.150	8.060	-1.957
1000	9.850	72.970	66.452	6.518	25.328	6.098	-1.333
1100	10.010	73.920	67.092	7.511	24.521	4.193	-.833
1200	10.170	74.800	67.699	8.521	23.731	2.395	-.436
1262	10.269	75.314	68.060	9.155	23.249	1.297	-.225

Phase changes: 722.65 K, melting point of Te; $\Delta H°$ = 4.180 kcal/mol.
1262 K, boiling point of Te to equilibrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15–2000 K: $Cp° = 8.599 + 1.186\times10^{-3}T - 0.242\times10^{5}T^{-2}$

$H°- H°_{298} = 8.599\times10^{-3}T + 0.593\times10^{-6}T^{2} + 0.242\times10^{2}T^{-1} - 2.698$

Formation equations (kcal/mol):

298.15–722.65 K: $\Delta Hf° = 38.789 - 0.431\times10^{-3}T - 4.781\times10^{-6}T^{2} + 28.200T^{-1}$

$\Delta Gf° = 38.789 + 0.431\times10^{-3}T\ln T + 4.781\times10^{-6}T^{2} + 14.100T^{-1} - 43.689\times10^{-3}T$

722.65–1262 K: $\Delta Hf° = 34.110 - 9.401\times10^{-3}T + 0.593\times10^{-6}T^{2} + 24.200T^{-1}$

$\Delta Gf° = 34.110 + 9.401\times10^{-3}T\ln T - 0.593\times10^{-6}T^{2} + 12.100T^{-1} - 92.376\times10^{-3}T$

Source: Data from Mills (158).

$Te_2(g)$

Tellurium (ideal diatomic gas)

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	8.680	61.870	61.870	0
300	8.680	61.920	61.870	.016
400	8.870	64.450	62.212	.895
500	9.050	66.450	62.868	1.791
600	9.210	68.120	63.613	2.704
700	9.370	69.550	64.360	3.633
800	9.540	70.810	65.086	4.579
900	9.700	71.940	65.784	5.540
1000	9.850	72.970	66.452	6.518
1100	10.010	73.920	67.092	7.511
1200	10.170	74.800	67.699	8.521
1300	10.330	75.620	68.277	9.546
1400	10.490	76.390	68.828	10.587
1500	10.450	77.110	69.355	11.632
1600	10.430	77.780	69.857	12.676
1700	10.410	78.420	70.351	13.718
1800	10.370	79.010	70.812	14.757
1900	10.330	79.570	71.258	15.792
2000	10.280	80.100	71.689	16.822

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.599 + 1.186\times10^{-3}T - 0.242\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.599\times10^{-3}T + 0.593\times10^{-6}T^2 + 0.242\times10^{2}T^{-1} - 2.698$

Source: Data from Mills (158).

$TeO_2(c,l)$

Tellurium Dioxide

[Formation: $Te(c,l) + O_2(g) = TeO_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.100	19.000	19.000	0	-77.100	-64.612	47.361
300	15.138	19.094	19.001	.028	-77.096	-64.533	47.012
400	16.513	23.661	19.613	1.619	-76.857	-60.381	32.990
500	17.238	27.431	20.811	3.310	-76.591	-56.291	24.604
600	17.703	30.617	22.187	5.058	-76.345	-52.255	19.034
700	18.046	33.373	23.593	6.846	-76.135	-48.259	15.067
722.65	18.109	33.949	23.909	7.255	-76.096	-47.358	14.322
722.65	18.109	33.949	23.909	7.255	-80.276	-47.358	14.322
800	18.325	35.802	24.971	8.665	-80.180	-43.846	11.978
900	18.565	37.974	26.296	10.510	-80.049	-39.310	9.546
1000	18.782	39.941	27.564	12.377	-79.909	-34.790	7.603
1006	18.794	40.054	27.638	12.490	-79.900	-34.520	7.499
1006	27.600	46.773	27.638	19.250	-73.140	-34.520	7.499
1100	27.600	49.239	29.381	21.844	-72.181	-30.963	6.152
1200	27.600	51.640	31.137	24.604	-71.169	-27.251	4.963
1262	27.600	53.031	32.179	26.315	-70.546	-25.004	4.330

*Heat capacity at 298 K estimated.

Phase changes: 722.65 K, melting point of Te; $\Delta H°$ = 4.180 kcal/mol.
1006 K, melting point of TeO_2; $\Delta H°$ = 6.760 kcal/mol.
1262 K, boiling point of Te to equilibrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1006 K: $Cp° = 17.438 + 1.596\times10^{-3}T - 2.502\times10^{5}T^{-2}$

$H°- H°_{298} = 17.438\times10^{-3}T + 0.798\times10^{-6}T^{2} + 2.502\times10^{2}T^{-1} - 6.109$

1006-1500 K: $Cp° = 27.600$

$H°- H°_{298} = 27.600\times10^{-3}T - 8.516$

Formation equations (kcal/mol):

298.15-722.65 K: $\Delta Hf° = -79.279 + 5.693\times10^{-3}T - 2.392\times10^{-6}T^{2} + 207.000T^{-1}$

$\Delta Gf° = -79.279 - 5.693\times10^{-3}T\ln T + 2.392\times10^{-6}T^{2} + 103.500T^{-1} + 79.752\times10^{-3}T$

722.65-1006 K: $\Delta Hf° = -81.618 + 1.208\times10^{-3}T + 0.295\times10^{-6}T^{2} + 205.000T^{-1}$

$\Delta Gf° = -81.618 - 1.208\times10^{-3}T\ln T - 0.295\times10^{-6}T^{2} + 102.500T^{-1} + 55.409\times10^{-3}T$

1006-1262 K: $\Delta Hf° = -84.025 + 11.370\times10^{-3}T - 0.503\times10^{-6}T^{2} - 45.200T^{-1}$

$\Delta Gf° = -84.025 - 11.370\times10^{-3}T\ln T + 0.503\times10^{-6}T^{2} - 22.600T^{-1} + 127.379\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (236). Heat capacity at 298 K estimated. High-temperature data based on Prescher (186) and Mezaki (154).

$TeO_2(c,l)$

Tellurium Dioxide

[Reaction: $0.5Te_2(g) + O_2(g) = TeO_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log K
	$C_p°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta H°$	$\Delta G°$	
298.15*	15.100	19.000	19.000	0	-96.265	-78.096	57.245
300	15.138	19.094	19.001	.028	-96.258	-77.984	56.810
400	16.513	23.661	19.613	1.619	-95.816	-71.955	39.314
500	17.238	27.431	20.811	3.310	-95.305	-66.047	28.869
600	17.703	30.617	22.187	5.058	-94.768	-60.244	21.944
700	18.046	33.373	23.593	6.846	-94.222	-54.534	17.026
800	18.325	35.802	24.971	8.665	-93.674	-48.904	13.360
900	18.565	37.974	26.296	10.510	-93.124	-43.340	10.524
1000	18.782	39.941	27.564	12.377	-92.573	-37.839	8.270
1006	18.794	40.054	27.638	12.490	-92.540	-37.510	8.149
1006	27.600	46.773	27.638	19.250	-85.780	-37.510	8.149
1100	27.600	49.239	29.381	21.844	-84.442	-33.059	6.568
1200	27.600	51.640	31.137	24.604	-83.035	-28.449	5.181
1300	27.600	53.850	32.801	27.364	-81.643	-23.958	4.028
1400	27.600	55.895	34.378	30.124	-80.268	-19.573	3.055
1500	27.600	57.799	35.876	32.884	-78.900	-15.287	2.227

*Heat capacity at 298 K estimated.

Phase change: 1006 K, melting point of TeO_2; $\Delta H°$ = 6.760 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1006 K: $C_p° = 17.438 + 1.596\times10^{-3}T - 2.502\times10^{5}T^{-2}$

$H°- H°_{298} = 17.438\times10^{-3}T + 0.798\times10^{-6}T^2 + 2.502\times10^{2}T^{-1} - 6.109$

1006-1500 K: $C_p° = 27.600$

$H°- H°_{298} = 27.600\times10^{-3}T - 8.516$

Reaction equations (kcal/mol):

298.15-1006 K: $\Delta H° = -98.673 + 5.908\times10^{-3}T - 0.001\times10^{-6}T^2 + 192.900T^{-1}$

$\Delta G° = -98.673 - 5.908\times10^{-3}T\ln T + 0.001\times10^{-6}T^2 + 96.450T^{-1} + 101.597\times10^{-3}T$

1006-1500 K: $\Delta H° = -101.080 + 16.070\times10^{-3}T - 0.799\times10^{-6}T^2 - 57.300T^{-1}$

$\Delta G° = -101.080 - 16.070\times10^{-3}T\ln T + 0.799\times10^{-6}T^2 - 28.650T^{-1} + 173.567\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (236). Heat capacity at 298 K estimated. High-temperature data based on Prescher (186) and Mezaki (154).

$TeO_2(g)$

Tellurium Dioxide (ideal gas)

[Formation: $Te(c,l) + O_2(g) = TeO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.813	65.520	65.520	0	-15.100	-16.482	12.081
300	10.832	65.590	65.523	.020	-15.104	-16.490	12.013
400	11.718	68.830	65.955	1.150	-15.326	-16.918	9.243
500	12.320	71.510	66.802	2.354	-15.547	-17.287	7.556
600	12.722	73.800	67.788	3.607	-15.796	-17.616	6.416
700	12.997	75.780	68.789	4.894	-16.087	-17.896	5.587
722.65	13.040	76.195	69.014	5.189	-16.162	-17.954	5.430
722.65	13.040	76.195	69.014	5.189	-20.342	-17.954	5.430
800	13.189	77.530	69.775	6.204	-20.641	-17.689	4.832
900	13.328	79.090	70.723	7.530	-21.029	-17.295	4.200
1000	13.431	80.500	71.631	8.869	-21.417	-16.857	3.684
1100	13.510	81.790	72.503	10.216	-21.809	-16.397	3.258
1200	13.571	82.970	73.328	11.570	-22.203	-15.881	2.892
1262	13.601	83.646	73.810	12.413	-22.448	-15.542	2.692

Phase changes: 722.65 K, melting point of Te; $\Delta H° = 4.180$ kcal/mol.
1262 K, boiling point of Te to equilbrium mixture.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 12.516 + 1.044\times10^{-3}T - 1.790\times10^{5}T^{-2}$

$H°- H°_{298} = 12.516\times10^{-3}T + 0.522\times10^{-6}T^2 + 1.790\times10^{2}T^{-1} - 4.378$

Formation equations (kcal/mol):

298.15-722.65 K: $\Delta Hf° = -15.548 + 0.771\times10^{-3}T - 2.668\times10^{-6}T^2 + 135.800T^{-1}$

$\Delta Gf° = -15.548 - 0.771\times10^{-3}T\ln T + 2.668\times10^{-6}T^2 + 67.900T^{-1} - 0.298\times10^{-3}T$

722.65-1262 K: $\Delta Hf° = -17.888 - 3.714\times10^{-3}T + 0.019\times10^{-6}T^2 + 133.800T^{-1}$

$\Delta Gf° = -17.888 + 3.714\times10^{-3}T\ln T - 0.019\times10^{-6}T^2 + 66.900T^{-1} - 24.642\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Muenow (164). All other data from Spoliti (210).

$TeO_2(g)$

Tellurium Dioxide (ideal gas)

[Reaction: $0.5Te_2(g) + O_2(g) = TeO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log K
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔH°	ΔG°	
298.15	10.813	65.520	65.520	0	-34.265	-29.966	21.965
300	10.832	65.590	65.523	.020	-34.266	-29.940	21.811
400	11.718	68.830	65.955	1.150	-34.286	-28.492	15.567
500	12.320	71.510	66.802	2.354	-34.261	-27.043	11.820
600	12.722	73.800	67.788	3.607	-34.219	-25.605	9.326
700	12.997	75.780	68.789	4.894	-34.174	-24.171	7.546
800	13.189	77.530	69.775	6.204	-34.136	-22.748	6.214
900	13.328	79.090	70.723	7.530	-34.104	-21.325	5.178
1000	13.431	80.500	71.631	8.869	-34.081	-19.906	4.350
1100	13.510	81.790	72.503	10.216	-34.070	-18.493	3.674
1200	13.571	82.970	73.328	11.570	-34.069	-17.079	3.110
1300	13.619	84.050	74.104	12.930	-34.077	-15.652	2.631
1400	13.658	85.060	74.850	14.294	-34.098	-14.234	2.222
1500	13.689	86.010	75.569	15.661	-34.123	-12.826	1.869

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 12.516 + 1.044\times10^{-3}T - 1.790\times10^{5}T^{-2}$

$H°- H°_{298} = 12.516\times10^{-3}T + 0.522\times10^{-6}T^{2} + 1.790\times10^{2}T^{-1} - 4.378$

Reaction equations (kcal/mol):

298.15-1500 K: $\Delta H° = -34.943 + 0.986\times10^{-3}T - 0.277\times10^{-6}T^{2} + 121.700T^{-1}$

$\Delta G° = -34.943 - 0.986\times10^{-3}T\ln T + 0.277\times10^{-6}T^{2} + 60.850T^{-1} + 21.546\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Muenow (164). All other data from Spoliti (210).

Th(c,1)

Thorium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.532	12.760	12.760	0
300	6.536	12.800	12.760	.012
400	6.761	14.712	13.019	.677
500	6.969	16.243	13.515	1.364
600	7.171	17.532	14.080	2.071
700	7.369	18.652	14.655	2.798
800	7.564	19.649	15.219	3.544
900	7.758	20.551	15.761	4.311
1000	7.950	21.378	16.282	5.096
1100	8.140	22.145	16.781	5.900
1200	8.329	22.861	17.258	6.724
1300	8.517	23.536	17.716	7.566
1400	8.704	24.174	18.155	8.427
1500	8.890	24.780	18.575	9.307
1600	9.075	25.360	18.982	10.205
1633	9.135	25.546	19.113	10.506
1633	8.420	26.073	19.113	11.366
1700	8.612	26.415	19.394	11.936
1800	8.898	26.915	19.797	12.812
1900	9.184	27.404	20.185	13.716
2000	9.470	27.882	20.558	14.649
2023	9.536	27.991	20.642	14.867
2023	11.000	29.622	20.642	18.167
2100	11.000	30.033	20.979	19.014
2200	11.000	30.545	21.402	20.114
2300	11.000	31.034	21.811	21.214
2400	11.000	31.502	22.205	22.314
2500	11.000	31.951	22.585	23.414

Phase changes: 1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.
2023 K, melting point of Th; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1633 K: $Cp^\circ = 6.058 + 1.894\times10^{-3}T - 0.079\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.058\times10^{-3}T + 0.947\times10^{-6}T^2 + 0.079\times10^{2}T^{-1} - 1.917$

1633-2023 K: $Cp^\circ = 3.809 + 2.836\times10^{-3}T - 0.535\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 3.809\times10^{-3}T + 1.418\times10^{-6}T^2 + 0.535\times10^{2}T^{-1} + 1.332$

2023-2500 K: $Cp^\circ = 11.000$

$H^\circ - H^\circ_{298} = 11.000\times10^{-3}T - 4.086$

Source: Data from Oetting (167).

Th(g)

Thorium (ideal monatomic gas)

[Formation: Th(c,1) = Th(g)]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	4.969	45.425	45.425	0	142.730	132.991	-97.484
300	4.969	45.456	45.426	.009	142.727	132.930	-96.838
400	4.982	46.886	45.618	.507	142.560	129.690	-70.859
500	5.039	48.003	45.989	1.007	142.373	126.493	-55.289
600	5.171	48.932	46.404	1.517	142.176	123.336	-44.925
700	5.388	49.745	46.825	2.044	141.976	120.211	-37.531
800	5.679	50.482	47.236	2.597	141.783	117.117	-31.994
900	6.024	51.171	47.635	3.182	141.601	114.043	-27.693
1000	6.398	51.825	48.022	3.803	141.437	110.990	-24.257
1100	6.780	52.452	48.396	4.462	141.292	107.954	-21.448
1200	7.154	53.059	48.760	5.159	141.165	104.927	-19.110
1300	7.509	53.645	49.113	5.892	141.056	101.914	-17.133
1400	7.838	54.214	49.458	6.659	140.962	98.906	-15.440
1500	8.138	54.765	49.793	7.458	140.881	95.903	-13.973
1600	8.409	55.299	50.120	8.286	140.811	92.909	-12.691
1633	8.490	55.471	50.227	8.565	140.789	91.921	-12.302
1633	8.490	55.471	50.227	8.565	139.929	91.921	-12.302
1700	8.653	55.816	50.440	9.139	139.933	89.951	-11.564
1800	8.871	56.317	50.753	10.016	139.934	87.010	-10.564
1900	9.065	56.802	51.058	10.913	139.927	84.071	-9.670
2000	9.238	57.272	51.358	11.828	139.909	81.129	-8.865
2023	9.274	57.378	51.426	12.041	139.904	80.454	-8.692
2023	9.274	57.378	51.426	12.041	136.604	80.454	-8.692
2100	9.393	57.726	51.650	12.760	136.476	78.321	-8.151
2200	9.532	58.167	51.937	13.706	136.322	75.554	-7.505
2300	9.657	58.593	52.216	14.666	136.182	72.796	-6.917
2400	9.770	59.007	52.492	15.637	136.053	70.041	-6.378
2500	9.873	59.408	52.760	16.620	135.936	67.293	-5.883

Phase changes: 1633 K, α - β transition point of Th; $\Delta H° = 0.860$ kcal/mol.
2023 K, melting point of Th; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 3.261 + 3.050\times10^{-3}T + 0.710\times10^{5}T^{-2}$

$H°-H°_{298} = 3.261\times10^{-3}T + 1.525\times10^{-6}T^{2} - 0.710\times10^{2}T^{-1} - 0.870$

Formation equations (kcal/mol):

298.15-1633 K: $\Delta Hf° = 143.777 - 2.797\times10^{-3}T + 0.578\times10^{-6}T^{2} - 78.900T^{-1}$

$\Delta Gf° = 143.777 + 2.797\times10^{-3}T\ln T - 0.578\times10^{-6}T^{2} - 39.450T^{-1} - 51.497\times10^{-3}T$

1633-2023 K: $\Delta Hf° = 140.528 - 0.548\times10^{-3}T + 0.107\times10^{-6}T^{2} - 124.500T^{-1}$

$\Delta Gf° = 140.528 + 0.548\times10^{-3}T\ln T - 0.107\times10^{-6}T^{2} - 62.250T^{-1} - 33.630\times10^{-3}T$

2023-2500 K: $\Delta Hf° = 145.946 - 7.739\times10^{-3}T + 1.525\times10^{-6}T^{2} - 71.000T^{-1}$

$\Delta Gf° = 145.946 + 7.739\times10^{-3}T\ln T - 1.525\times10^{-6}T^{2} - 35.500T^{-1} - 88.186\times10^{-3}$

Source: Data from Oetting (167).

ThO(g)

Thorium Oxide (ideal gas)

[Formation: $Th(c,l) + 0.5O_2(g) = ThO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.473	57.351	57.351	0	-6.077	-12.066	8.845
300	7.481	57.397	57.351	.014	-6.082	-12.103	8.817
400	7.864	59.604	57.649	.782	-6.333	-14.072	7.689
500	8.150	61.391	58.225	1.583	-6.585	-15.979	6.984
600	8.353	62.896	58.881	2.409	-6.844	-17.833	6.496
700	8.501	64.195	59.549	3.252	-7.117	-19.643	6.133
800	8.621	65.339	60.204	4.108	-7.406	-21.413	5.850
900	8.732	66.361	60.832	4.976	-7.712	-23.147	5.621
1000	8.845	67.286	61.431	5.855	-8.031	-24.844	5.430
1100	8.966	68.135	62.003	6.745	-8.365	-26.509	5.267
1200	9.099	68.921	62.548	7.648	-8.710	-28.145	5.126
1300	9.243	69.655	63.067	8.565	-9.063	-29.749	5.001
1400	9.395	70.345	63.561	9.497	-9.424	-31.326	4.890
1500	9.552	70.999	64.036	10.445	-9.791	-32.879	4.790
1600	9.712	71.620	64.490	11.408	-10.164	-34.405	4.699
1633	9.765	71.819	64.636	11.729	-10.289	-34.903	4.671
1633	9.765	71.819	64.636	11.729	-11.149	-34.903	4.671
1700	9.873	72.214	64.928	12.387	-11.357	-35.874	4.612
1800	10.031	72.782	65.348	13.382	-11.682	-37.307	4.530
1900	10.187	73.329	65.754	14.393	-12.022	-38.722	4.454
2000	10.339	73.855	66.146	15.419	-12.379	-40.119	4.384
2023	10.373	73.973	66.234	15.657	-12.462	-40.436	4.368
2023	10.373	73.973	66.234	15.657	-15.762	-40.436	4.368
2100	10.487	74.363	66.524	16.461	-16.154	-41.367	4.305
2200	10.630	74.855	66.893	17.517	-16.653	-42.557	4.228
2300	10.767	75.330	67.249	18.587	-17.141	-43.722	4.154
2400	10.901	75.791	67.595	19.670	-17.618	-44.868	4.086
2500	11.029	76.239	67.932	20.767	-18.085	-45.994	4.021

Phase changes: 1633 K, α - β transition point of Th; $\Delta H° = 0.860$ kcal/mol.
2023 K, melting point of Th; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 7.647 + 1.312\times10^{-3}T - 0.503\times10^{5}T^{-2}$

$H°- H°_{298} = 7.647\times10^{-3}T + 0.656\times10^{-6}T^{2} + 0.503\times10^{2}T^{-1} - 2.507$

Formation equations (kcal/mol):

298.15-1633 K: $\Delta Hf° = -5.491 - 2.026\times10^{-3}T - 0.542\times10^{-6}T^{2} + 19.800T^{-1}$

$\Delta Gf° = -5.491 + 2.026\times10^{-3}T\ln T + 0.542\times10^{-6}T^{2} + 9.900T^{-1} - 33.870\times10^{-3}T$

1633-2000 K: $\Delta Hf° = -8.740 + 0.223\times10^{-3}T - 1.013\times10^{-6}T^{2} - 25.800T^{-1}$

$\Delta Gf° = -8.740 - 0.223\times10^{-3}T\ln T + 1.013\times10^{-6}T^{2} - 12.900T^{-1} - 16.003\times10^{-3}T$

2000-2023 K: $\Delta Hf° = -8.072 - 0.332\times10^{-3}T - 0.867\times10^{-6}T^{2} - 318.200T^{-1}$

$\Delta Gf° = -8.072 + 0.332\times10^{-3}T\ln T + 0.867\times10^{-6}T^{2} - 159.100T^{-1} - 20.225\times10^{-3}T$

2023-2500 K: $\Delta Hf° = -2.654 - 7.523\times10^{-3}T + 0.552\times10^{-6}T^{2} - 264.700T^{-1}$

$\Delta Gf° = -2.654 + 7.523\times10^{-3}T\ln T - 0.552\times10^{-6}T^{2} - 132.350T^{-1} - 74.781\times10^{-3}T$

Source: Data from Wagman (240).

$ThO_2(c)$

Thorium Dioxide

[Formation: $Th(c,1) + O_2(g) = ThO_2(c)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.770	15.590	15.590	0	-293.120	-279.353	204.769
300	14.810	15.680	15.590	.027	-293.118	-279.267	203.443
400	16.210	20.160	16.192	1.587	-292.933	-274.676	150.074
500	16.960	23.860	17.364	3.248	-292.690	-270.138	118.076
600	17.440	27.000	18.717	4.970	-292.430	-265.653	96.763
700	17.810	29.720	20.101	6.733	-292.172	-261.212	81.553
800	18.110	32.120	21.457	8.530	-291.919	-256.808	70.156
900	18.370	34.260	22.756	10.354	-291.676	-252.427	61.297
1000	18.610	36.210	24.006	12.204	-291.438	-248.080	54.217
1100	18.840	38.000	25.203	14.077	-291.208	-243.760	48.430
1200	19.050	39.650	26.341	15.971	-290.986	-239.459	43.611
1300	19.260	41.180	27.421	17.887	-290.768	-235.168	39.535
1400	19.460	42.610	28.451	19.823	-290.557	-230.893	36.044
1500	19.660	43.960	29.441	21.779	-290.351	-226.642	33.021
1600	19.850	45.240	30.394	23.754	-290.151	-222.409	30.379
1633	19.913	45.646	30.698	24.410	-290.086	-221.012	29.578
1633	19.913	45.646	30.698	24.410	-290.946	-221.012	29.578
1700	20.040	46.450	31.304	25.749	-290.769	-218.147	28.044
1800	20.230	47.600	32.176	27.763	-290.519	-213.880	25.968
1900	20.420	48.700	33.018	29.796	-290.284	-209.631	24.113
2000	20.610	49.750	33.826	31.847	-290.065	-205.389	22.444
2023	20.654	49.986	34.009	32.322	-290.016	-204.414	22.083
2023	20.654	49.986	34.009	32.322	-293.316	-204.414	22.083
2100	20.800	50.760	34.609	33.917	-293.265	-201.031	20.921
2200	20.980	51.730	35.364	36.006	-293.186	-196.637	19.534
2300	21.170	52.670	36.099	38.114	-293.094	-192.257	18.268
2400	21.350	53.570	36.804	40.239	-292.990	-187.865	17.107
2500	21.530	54.450	37.496	42.384	-292.871	-183.498	16.041

Phase changes: 1633 K, α - β transition point of Th; $\Delta H° = 0.860$ kcal/mol.
2023 K, melting point of Th; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 17.058 + 1.808\times10^{-3}T - 2.513\times10^{5}T^{-2}$

$H°- H°_{298} = 17.058\times10^{-3}T + 0.904\times10^{-6}T^{2} + 2.513\times10^{2}T^{-1} - 6.009$

Formation equations (kcal/mol):

298.15-1633 K: $\Delta Hf° = -294.860 + 3.770\times10^{-3}T - 0.546\times10^{-6}T^{2} + 198.200T^{-1}$

$\Delta Gf° = -294.860 - 3.770\times10^{-3}T\ln T + 0.546\times10^{-6}T^{2} + 99.100T^{-1} + 72.214\times10^{-3}T$

1633-2000 K: $\Delta Hf° = -298.109 + 6.019\times10^{-3}T - 1.017\times10^{-6}T^{2} + 152.600T^{-1}$

$\Delta Gf° = -298.109 - 6.019\times10^{-3}T\ln T + 1.017\times10^{-6}T^{2} + 76.300T^{-1} + 90.082\times10^{-3}T$

2000-2023 K: $\Delta Hf° = -296.773 + 4.909\times10^{-3}T - 0.723\times10^{-6}T^{2} - 432.200T^{-1}$

$\Delta Gf° = -296.773 - 4.909\times10^{-3}T\ln T + 0.723\times10^{-6}T^{2} - 216.100T^{-1} + 81.637\times10^{-3}T$

2023-2500 K: $\Delta Hf° = -291.355 - 2.282\times10^{-3}T + 0.695\times10^{-6}T^{2} - 378.700T^{-1}$

$\Delta Gf° = -291.355 + 2.282\times10^{-3}T\ln T - 0.695\times10^{-6}T^{2} - 189.350T^{-1} + 27.081\times10^{-3}T$

Source: Data from Wagman (240).

$ThO_2(g)$

Thorium Dioxide (ideal gas)

[Formation: $Th(c,l) + O_2(g) = ThO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.317	68.701	68.701	0	-118.670	-120.738	88.502
300	11.334	68.771	68.701	.021	-118.674	-120.751	87.966
400	12.110	72.145	69.155	1.196	-118.874	-121.411	66.335
500	12.621	74.906	70.038	2.434	-119.054	-122.025	53.336
600	12.955	77.239	71.049	3.714	-119.236	-122.602	44.657
700	13.180	79.254	72.080	5.022	-119.433	-123.147	38.448
800	13.336	81.025	73.090	6.348	-119.651	-123.664	33.783
900	13.448	82.602	74.061	7.687	-119.893	-124.152	30.148
1000	13.531	84.024	74.988	9.036	-120.156	-124.612	27.234
1100	13.593	85.316	75.868	10.393	-120.442	-125.041	24.843
1200	13.642	86.501	76.706	11.754	-120.753	-125.447	22.847
1300	13.680	87.595	77.502	13.121	-121.084	-125.824	21.153
1400	13.711	88.610	78.260	14.490	-121.440	-126.176	19.697
1500	13.736	89.557	78.982	15.863	-121.817	-126.503	18.431
1600	13.757	90.444	79.671	17.237	-122.218	-126.802	17.320
1633	13.763	90.725	79.891	17.691	-122.355	-126.895	16.983
1633	13.763	90.725	79.891	17.691	-123.215	-126.895	16.983
1700	13.774	91.278	80.329	18.614	-123.454	-127.039	16.332
1800	13.788	92.066	80.959	19.992	-123.840	-127.240	15.449
1900	13.801	92.812	81.564	21.372	-124.258	-127.418	14.656
2000	13.811	93.520	82.144	22.752	-124.710	-127.574	13.940
2023	13.813	93.678	82.274	23.070	-124.818	-127.605	13.785
2023	13.813	93.678	82.274	23.070	-128.118	-127.605	13.785
2100	13.820	94.194	82.702	24.134	-128.598	-127.575	13.277
2200	13.828	94.837	83.239	25.516	-129.226	-127.512	12.667
2300	13.835	95.452	83.757	26.899	-129.859	-127.421	12.108
2400	13.841	96.041	84.256	28.283	-130.496	-127.302	11.592
2500	13.846	96.606	84.739	29.667	-131.138	-127.155	11.116

Phase changes: 1633 K, α - β transition point of Th; $\Delta H° = 0.860$ kcal/mol.
2023 K, melting point of Th; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 13.318 + 0.300\times10^{-3}T - 1.858\times10^{5}T^{-2}$

$H°- H°_{298} = 13.318\times10^{-3}T + 0.150\times10^{-6}T^{2} + 1.858\times10^{2}T^{-1} - 4.607$

Formation equations (kcal/mol):

298.15-1633 K: $\Delta Hf° = -119.008 + 0.030\times10^{-3}T - 1.300\times10^{-6}T^{2} + 132.700T^{-1}$

$\Delta Gf° = -119.008 - 0.030\times10^{-3}T\ln T + 1.300\times10^{-6}T^{2} + 66.350T^{-1} - 6.764\times10^{-3}T$

1633-2000 K: $\Delta Hf° = -122.257 + 2.279\times10^{-3}T - 1.771\times10^{-6}T^{2} + 87.100T^{-1}$

$\Delta Gf° = -122.257 - 2.279\times10^{-3}T\ln T + 1.771\times10^{-6}T^{2} + 43.550T^{-1} + 11.103\times10^{-3}T$

2000-2023 K: $\Delta Hf° = -120.921 + 1.169\times10^{-3}T - 1.477\times10^{-6}T^{2} - 497.700T^{-1}$

$\Delta Gf° = -120.921 - 1.169\times10^{-3}T\ln T + 1.477\times10^{-6}T^{2} - 248.850T^{-1} + 2.659\times10^{-3}T$

2023-2500 K: $\Delta Hf° = -115.503 - 6.022\times10^{-3}T - 0.059\times10^{-6}T^{2} - 444.200T^{-1}$

$\Delta Gf° = -115.503 + 6.022\times10^{-3}T\ln T + 0.059\times10^{-6}T^{2} - 222.100T^{-1} - 51.897\times10^{-3}T$

Source: Data from Wagman (240).

Ti(c,l)

Titanium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.980	7.320	7.320	0
300	5.990	7.360	7.323	.011
400	6.310	9.130	7.563	.627
500	6.530	10.560	8.020	1.270
600	6.770	11.770	8.547	1.934
700	7.010	12.840	9.093	2.623
800	7.250	13.790	9.620	3.336
900	7.480	14.660	10.133	4.074
1000	7.710	15.460	10.628	4.832
1100	7.950	16.200	11.095	5.615
1156	8.100	16.600	11.355	6.063
1156	6.995	17.480	11.355	7.080
1200	7.098	17.743	11.585	7.390
1300	7.310	18.320	12.081	8.111
1400	7.507	18.869	12.546	8.852
1500	7.708	19.394	12.986	9.612
1600	7.932	19.898	13.402	10.394
1700	8.198	20.387	13.799	11.200
1800	8.525	20.864	14.177	12.036
1900	8.932	21.336	14.542	12.908
1945	9.146	21.547	14.701	13.315
1945	11.050	23.244	14.701	16.615
2000	11.050	23.552	14.941	17.223
2100	11.050	24.091	15.363	18.328
2200	11.050	24.605	15.772	19.433
2300	11.050	25.097	16.167	20.538
2400	11.050	25.567	16.549	21.643
2500	11.050	26.018	16.919	22.748
2600	11.050	26.451	17.277	23.853
2700	11.050	26.868	17.624	24.958
2800	11.050	27.270	17.962	26.063
2900	11.050	27.658	18.290	27.168
3000	11.050	28.033	18.609	28.273

Phase changes: 1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.
3562 K, boiling point of Ti; ΔH° = 100.6 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1156 K:

$$Cp^\circ = 5.477 + 2.246\times10^{-3}T - 0.148\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 5.477\times10^{-3}T + 1.123\times10^{-6}T^2 + 0.148\times10^{2}T^{-1} - 1.782$$

1156-1945 K:

$$Cp^\circ = 3.077 + 2.892\times10^{-3}T + 7.681\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 3.077\times10^{-3}T + 1.446\times10^{-6}T^2 - 7.681\times10^{2}T^{-1} + 2.255$$

1945-3000 K:

$$Cp^\circ = 11.050$$

$$H^\circ - H^\circ_{298} = 11.050\times10^{-3}T - 4.877$$

Sources: Data from 298 K to 1156 K from Hultgren (99). Data 1156 K to 1945 K based on Hultgren (99) and Cezairliyan (27). Temperature of fusion from Cezairliyan (26). Enthalpy of fusion and data for Ti(liq) based on Treverton (224) and Berezin (17).

Ti(g)

Titanium (ideal monatomic gas)

[Formation: Ti(c,l) = Ti(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.839	43.066	43.066	0	113.000	102.342	-75.018
300	5.831	43.102	43.066	.011	113.000	102.277	-74.508
400	5.522	44.733	43.291	.577	112.950	98.709	-53.931
500	5.344	45.945	43.705	1.120	112.850	95.158	-41.593
600	5.237	46.909	44.162	1.648	112.714	91.631	-33.376
700	5.170	47.711	44.614	2.168	112.545	88.135	-27.517
800	5.128	48.398	45.044	2.683	112.347	84.661	-23.128
900	5.104	49.001	45.452	3.194	112.120	81.213	-19.721
1000	5.096	49.538	45.834	3.704	111.872	77.794	-17.002
1100	5.106	50.024	46.193	4.214	111.599	74.393	-14.780
1156	5.121	50.278	46.384	4.500	111.437	72.507	-13.708
1156	5.121	50.278	46.384	4.500	110.420	72.507	-13.708
1200	5.132	50.469	46.531	4.726	110.336	71.065	-12.943
1300	5.176	50.881	46.849	5.241	110.130	67.801	-11.398
1400	5.237	51.267	47.151	5.762	109.910	64.553	-10.077
1500	5.313	51.631	47.438	6.289	109.677	61.321	-8.934
1600	5.403	51.977	47.711	6.825	109.431	58.105	-7.937
1700	5.504	52.307	47.972	7.370	109.170	54.906	-7.059
1800	5.616	52.625	48.222	7.926	108.890	51.720	-6.280
1900	5.737	52.932	48.461	8.494	108.586	48.554	-5.585
1945	5.794	53.067	48.566	8.753	108.438	47.133	-5.296
1945	5.794	53.067	48.566	8.753	105.138	47.133	-5.296
2000	5.864	53.229	48.692	9.074	104.851	45.497	-4.972
2100	5.996	53.518	48.915	9.666	104.338	42.541	-4.427
2200	6.132	53.801	49.131	10.273	103.840	39.609	-3.935
2300	6.271	54.076	49.340	10.893	103.355	36.703	-3.488
2400	6.413	54.346	49.543	11.527	102.884	33.814	-3.079
2500	6.557	54.611	49.741	12.176	102.428	30.946	-2.705
2600	6.701	54.871	49.933	12.839	101.986	28.094	-2.361
2700	6.847	55.126	50.120	13.516	101.558	25.261	-2.045
2800	6.993	55.378	50.304	14.208	101.145	22.443	-1.752
2900	7.140	55.626	50.483	14.915	100.747	19.640	-1.480
3000	7.286	55.871	50.659	15.636	100.363	16.849	-1.227

Phase changes: 1156 K, α - β transition point of Ti; $\Delta H° = 1.017$ kcal/mol.
1945 K, melting point of Ti; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 4.561 + 0.598\times10^{-3}T + 0.977\times10^{5}T^{-2}$

$H°- H°_{298} = 4.561\times10^{-3}T + 0.299\times10^{-6}T^{2} - 0.977\times10^{2}T^{-1} - 1.059$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = 113.724 - 0.916\times10^{-3}T - 0.824\times10^{-6}T^{2} - 112.500T^{-1}$

$\Delta Gf° = 113.724 + 0.916\times10^{-3}T\ln T + 0.824\times10^{-6}T^{2} - 56.250T^{-1} - 43.005\times10^{-3}T$

1156-1945 K: $\Delta Hf° = 109.687 + 1.484\times10^{-3}T - 1.147\times10^{-6}T^{2} + 670.400T^{-1}$

$\Delta Gf° = 109.687 - 1.484\times10^{-3}T\ln T + 1.147\times10^{-6}T^{2} + 335.200T^{-1} - 23.253\times10^{-3}T$

1945-3000 K: $\Delta Hf° = 116.819 - 6.489\times10^{-3}T + 0.299\times10^{-6}T^{2} - 97.700T^{-1}$

$\Delta Gf° = 116.819 + 6.489\times10^{-3}T\ln T - 0.299\times10^{-6}T^{2} - 48.850T^{-1} - 84.385\times10^{-3}T$

Source: Data from JANAF (51).

TiO(g)

Titanium Oxide (ideal gas)

[Formation: $Ti(c,l) + 0.5O_2(g) = TiO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.762	55.776	55.776	0	13.000	5.858	-4.294
300	7.768	55.824	55.777	.014	12.997	5.815	-4.236
400	8.131	58.108	56.086	.809	12.821	3.447	-1.883
500	8.433	59.957	56.681	1.638	12.641	1.123	-0.491
600	8.646	61.514	57.359	2.493	12.455	-1.163	0.424
700	8.792	62.859	58.052	3.365	12.248	-3.411	1.065
800	8.894	64.040	58.728	4.250	12.022	-5.634	1.539
900	8.967	65.092	59.378	5.143	11.769	-7.826	1.900
1000	9.021	66.039	59.996	6.043	11.498	-9.986	2.182
1100	9.062	66.901	60.586	6.947	11.200	-12.127	2.409
1156	9.080	67.352	60.902	7.455	11.023	-13.307	2.516
1156	9.080	67.352	60.902	7.455	10.006	-13.307	2.516
1200	9.094	67.691	61.145	7.855	9.908	-14.192	2.585
1300	9.120	68.420	61.677	8.766	9.671	-16.191	2.722
1400	9.141	69.097	62.183	9.679	9.411	-18.172	2.837
1500	9.158	69.728	62.665	10.594	9.130	-20.131	2.933
1600	9.174	70.320	63.126	11.510	8.826	-22.074	3.015
1700	9.190	70.876	63.565	12.428	8.497	-23.993	3.085
1800	9.206	71.402	63.986	13.348	8.137	-25.896	3.144
1900	9.223	71.900	64.389	14.270	7.740	-27.774	3.195
1945	9.232	72.116	64.566	14.685	7.546	-28.613	3.215
1945	9.232	72.116	64.566	14.685	4.246	-28.613	3.215
2000	9.242	72.374	64.778	15.193	3.899	-29.539	3.228
2100	9.264	72.825	65.150	16.118	3.266	-31.195	3.246
2200	9.290	73.257	65.509	17.046	2.634	-32.822	3.261
2300	9.319	73.670	65.854	17.976	2.001	-34.417	3.270
2400	9.353	74.068	66.189	18.910	1.369	-35.989	3.277
2500	9.390	74.450	66.511	19.847	.738	-37.531	3.281
2600	9.433	74.819	66.824	20.788	.109	-39.051	3.282
2700	9.479	75.176	67.126	21.734	-.518	-40.545	3.282
2800	9.530	75.522	67.421	22.684	-1.143	-42.017	3.279
2900	9.585	75.857	67.705	23.640	-1.765	-43.463	3.275
3000	9.644	76.183	67.983	24.601	-2.385	-44.890	3.270

Phase changes: 1156 K, α - β transition point of Ti; $\Delta H° = 1.017$ kcal/mol.
1945 K, melting point of Ti; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 8.740 + 0.288\times10^{-3}T - 0.946\times10^{5}T^{-2}$

$H°- H°_{298} = 8.740\times10^{-3}T + 0.144\times10^{-6}T^{2} + 0.946\times10^{2}T^{-1} - 2.936$

TiO(g) - Continued

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf^\circ = 13.022 - 0.352\times10^{-3}T - 1.231\times10^{-6}T^2 + 57.200T^{-1}$

$\Delta Gf^\circ = 13.022 + 0.352\times10^{-3}T\ln T + 1.231\times10^{-6}T^2 + 28.600T^{-1} - 26.723\times10^{-3}T$

1156-1945 K: $\Delta Hf^\circ = 8.985 + 2.048\times10^{-3}T - 1.553\times10^{-6}T^2 + 840.100T^{-1}$

$\Delta Gf^\circ = 8.985 - 2.048\times10^{-3}T\ln T + 1.553\times10^{-6}T^2 + 420.050T^{-1} - 6.971\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = 16.118 - 5.925\times10^{-3}T - 0.107\times10^{-6}T^2 + 72.000T^{-1}$

$\Delta Gf^\circ = 16.118 + 5.925\times10^{-3}T\ln T + 0.107\times10^{-6}T^2 + 36.000T^{-1} - 68.103\times10^{-3}T$

2000-3000 K: $\Delta Hf^\circ = 16.786 - 6.480\times10^{-3}T + 0.040\times10^{-6}T^2 - 220.400T^{-1}$

$\Delta Gf^\circ = 16.786 + 6.480\times10^{-3}T\ln T - 0.040\times10^{-6}T^2 - 110.200T^{-1} - 72.325\times10^{-3}T$

Source: Data from Chase (33).

TiO_2(rutile)

Titanium Dioxide

[Formation: $Ti(c,l) + O_2(g) = TiO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.160	12.040	12.040	0	-225.670	-212.466	155.740
300	13.196	12.122	12.042	.024	-225.670	-212.384	154.720
400	14.893	16.167	12.580	1.435	-225.585	-207.964	113.625
500	16.051	19.623	13.651	2.986	-225.408	-203.579	88.983
600	16.804	22.622	14.904	4.631	-225.182	-199.235	72.570
700	17.261	25.249	16.196	6.337	-224.943	-194.922	60.857
800	17.519	27.573	17.477	8.077	-224.714	-190.652	52.083
900	17.662	29.645	18.715	9.837	-224.506	-186.405	45.265
1000	17.755	31.511	19.903	11.608	-224.320	-182.181	39.815
1100	17.845	33.208	21.037	13.388	-224.162	-177.982	35.361
1156	17.910	34.095	21.648	14.389	-224.083	-175.629	33.203
1156	17.910	34.095	21.648	14.389	-225.100	-175.629	33.203
1200	17.961	34.765	22.117	15.178	-224.995	-173.748	31.643
1300	18.116	36.209	23.147	16.981	-224.769	-169.488	28.493
1400	18.307	37.558	24.128	18.802	-224.553	-165.243	25.795
1500	18.524	38.828	25.065	20.644	-224.341	-161.013	23.459
1600	18.752	40.031	25.964	22.507	-224.137	-156.799	21.418
1700	18.976	41.175	26.826	24.394	-223.938	-152.596	19.617
1800	19.195	42.266	27.654	26.302	-223.754	-148.406	18.019
1900	19.425	43.309	28.450	28.233	-223.589	-144.222	16.589
1945	19.556	43.765	28.799	29.110	-223.523	-142.344	15.994
1945	19.556	43.765	28.799	29.110	-226.823	-142.344	15.994
2000	19.715	44.313	29.219	30.189	-226.847	-139.957	15.294

Phase changes: 1156 K, α ~ β transition point of Ti; $\Delta H°$ = 1.017 kcal/mol.
1945 K, melting point of Ti; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 16.914 + 1.220\times10^{-3}T - 3.661\times10^{5}T^{-2}$

$H°- H°_{298} = 16.914\times10^{-3}T + 0.610\times10^{-6}T^{2} + 3.661\times10^{2}T^{-1} - 6.325$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -227.861 + 4.207\times10^{-3}T - 1.016\times10^{-6}T^{2} + 306.100T^{-1}$

$\Delta Gf° = -227.861 - 4.207\times10^{-3}T\ln T + 1.016\times10^{-6}T^{2} + 153.050T^{-1} + 73.578\times10^{-3}T$

1156-1945 K: $\Delta Hf° = -231.898 + 6.607\times10^{-3}T - 1.339\times10^{-6}T^{2} + 1089.000T^{-1}$

$\Delta Gf° = -231.898 - 6.607\times10^{-3}T\ln T + 1.339\times10^{-6}T^{2} + 544.500T^{-1} + 93.330\times10^{-3}T$

1945-2000 K: $\Delta Hf° = -224.766 - 1.366\times10^{-3}T + 0.107\times10^{-6}T^{2} + 320.900T^{-1}$

$\Delta Gf° = -224.766 + 1.366\times10^{-3}T\ln T - 0.107\times10^{-6}T^{2} + 160.450T^{-1} + 32.197\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (37). Low-temperature heat capacities and entropy at 298 K from Shomate (198). High-temperature data based on Naylor (165).

TiO_2(anatase)

Titanium Dioxide

[Formation: $Ti(c) + O_2(g) = TiO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.220	11.930	11.930	0	-224.600	-211.364	154.932
300	13.277	12.012	11.930	.025	-224.599	-211.280	153.915
400	15.343	16.158	12.481	1.471	-224.479	-206.854	113.018
500	16.332	19.699	13.581	3.059	-224.265	-202.474	88.500
600	16.907	22.732	14.859	4.724	-224.019	-198.138	72.171
700	17.287	25.368	16.177	6.434	-223.776	-193.838	60.518
800	17.565	27.696	17.473	8.178	-223.543	-189.580	51.790
900	17.786	29.778	18.727	9.946	-223.327	-185.346	45.008
1000	17.972	31.662	19.928	11.734	-223.124	-181.136	39.587
1100	18.136	33.382	21.074	13.539	-222.941	-176.952	35.157
1156	18.221	34.285	21.693	14.557	-222.845	-174.611	33.011
1156	18.221	34.285	21.693	14.557	-223.862	-174.611	33.011
1200	18.287	34.967	22.167	15.360	-223.743	-172.738	31.460
1300*	18.429	36.436	23.208	17.196	-223.484	-168.498	28.327

*Anatase transforms irreversibly to rutile. Temperatures for this transition range from 917 K upwards. Apparently anatase is metastable with respect to rutile at all temperatures.

Phase change: 1156 K, α - β transition point of Ti; $\Delta H° = 1.017$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp° = 17.545 + 0.828\times10^{-3}T - 4.064\times10^{5}T^{-2}$

$H°- H°_{298} = 17.545\times10^{-3}T + 0.414\times10^{-6}T^2 + 4.064\times10^{2}T^{-1} - 6.631$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -227.097 + 4.838\times10^{-3}T - 1.212\times10^{-6}T^2 + 346.400T^{-1}$

$\Delta Gf° = -227.097 - 4.838\times10^{-3}T\ln T + 1.212\times10^{-6}T^2 + 173.200T^{-1} + 78.024\times10^{-3}T$

1156-1300 K: $\Delta Hf° = -231.134 + 7.238\times10^{-3}T - 1.535\times10^{-6}T^2 + 1129.300T^{-1}$

$\Delta Gf° = -231.134 - 7.238\times10^{-3}T\ln T + 1.535\times10^{-6}T^2 + 564.650T^{-1} + 97.776\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (238). Low-temperature heat capacities and entropy at 298 K from Shomate (198). High-temperature data based on Naylor (165).

$TiO_2(g)$

Titanium Dioxide (ideal gas)

[Formation: $Ti(c,l) + O_2(g) = TiO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.552	62.151	62.151	0	-73.000	-74.737	54.783
300	10.569	62.216	62.151	.020	-73.004	-74.746	54.452
400	11.419	65.378	62.575	1.121	-73.229	-75.292	41.137
500	12.050	67.998	63.406	2.296	-73.428	-75.787	33.126
600	12.495	70.236	64.363	3.524	-73.619	-76.240	27.770
700	12.808	72.188	65.344	4.791	-73.819	-76.655	23.933
800	13.033	73.913	66.309	6.083	-74.038	-77.048	21.048
900	13.198	75.458	67.241	7.395	-74.278	-77.409	18.797
1000	13.322	76.856	68.135	8.721	-74.537	-77.743	16.991
1100	13.417	78.130	68.985	10.059	-74.821	-78.055	15.508
1156	13.458	78.798	69.445	10.811	-74.991	-78.213	14.786
1156	13.458	78.798	69.445	10.811	-76.008	-78.213	14.786
1200	13.491	79.301	69.798	11.404	-76.099	-78.295	14.259
1300	13.550	80.383	70.571	12.756	-76.324	-78.469	13.192
1400	13.597	81.389	71.308	14.114	-76.571	-78.625	12.274
1500	13.636	82.328	72.011	15.475	-76.840	-78.762	11.475
1600	13.668	83.210	72.684	16.841	-77.133	-78.882	10.775
1700	13.695	84.039	73.328	18.209	-77.453	-78.980	10.153
1800	13.718	84.822	73.944	19.580	-77.806	-79.059	9.599
1900	13.737	85.565	74.538	20.952	-78.200	-79.120	9.101
1945	13.745	85.887	74.797	21.570	-78.393	-79.140	8.892
1945	13.745	85.887	74.797	21.570	-81.693	-79.140	8.892
2000	13.755	86.270	75.106	22.327	-82.039	-79.063	8.639
2100	13.770	86.941	75.654	23.703	-82.673	-78.897	8.211
2200	13.784	87.582	76.182	25.081	-83.310	-78.703	7.818
2300	13.797	88.195	76.691	26.460	-83.952	-78.478	7.457
2400	13.810	88.783	77.183	27.840	-84.598	-78.228	7.124
2500	13.822	89.347	77.658	29.222	-85.247	-77.950	6.814
2600	13.835	89.889	78.118	30.605	-85.900	-77.645	6.527
2700	13.849	90.411	78.563	31.989	-86.557	-77.315	6.258
2800	13.864	90.915	78.995	33.375	-87.217	-76.958	6.007
2900	13.879	91.402	79.415	34.762	-87.881	-76.580	5.771
3000	13.897	91.873	79.823	36.150	-88.549	-76.180	5.550

Phase changes: 1156 K, α - β transition point of Ti; $\Delta H°$ = 1.017 kcal/mol.
1945 K, melting point of Ti; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 12.667 + 0.642\times10^{-3}T - 2.050\times10^{5}T^{-2}$

$H°- H°_{298} = 12.667\times10^{-3}T + 0.321\times10^{-6}T^{2} + 2.050\times10^{2}T^{-1} - 4.493$

$TiO_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -73.358 - 0.040\times10^{-3}T - 1.305\times10^{-6}T^2 + 145.000T^{-1}$

$\Delta Gf° = -73.358 + 0.040\times10^{-3}T\ln T + 1.305\times10^{-6}T^2 + 72.500T^{-1} - 6.056\times10^{-3}T$

1156-1945 K: $\Delta Hf° = -77.395 + 2.360\times10^{-3}T - 1.628\times10^{-6}T^2 + 927.900T^{-1}$

$\Delta Gf° = -77.395 - 2.360\times10^{-3}T\ln T + 1.628\times10^{-6}T^2 + 463.950T^{-1} + 13.696\times10^{-3}T$

1945-2000 K: $\Delta Hf° = -70.263 - 5.613\times10^{-3}T - 0.182\times10^{-6}T^2 + 159.800T^{-1}$

$\Delta Gf° = -70.263 + 5.613\times10^{-3}T\ln T + 0.182\times10^{-6}T^2 + 79.900T^{-1} - 47.437\times10^{-3}T$

2000-3000 K: $\Delta Hf° = -68.927 - 6.723\times10^{-3}T + 0.112\times10^{-6}T^2 - 425.000T^{-1}$

$\Delta Gf° = -68.927 + 6.723\times10^{-3}T\ln T - 0.112\times10^{-6}T^2 - 212.500T^{-1} - 55.881\times10^{-3}T$

Source: Data from Chase (33).

$Ti_2O_3(c)$

Dititanium Trioxide

[Formation: $2Ti(c,l) + 1.5O_2(g) = Ti_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	22.910	18.480	18.480	0	-363.500	-342.729	251.224
300	23.071	18.622	18.482	.042	-363.500	-342.598	249.579
400	28.911	26.076	19.456	2.648	-363.190	-335.663	183.395
473	32.191	31.207	20.879	4.885	-362.685	-330.684	152.791
473	30.880	31.662	20.879	5.100	-362.470	-330.684	152.791
500	31.344	33.389	21.507	5.941	-362.280	-328.874	143.749
600	32.620	39.225	23.985	9.144	-361.537	-322.261	117.382
700	33.474	44.322	26.535	12.451	-360.776	-315.764	98.585
800	34.094	48.834	29.045	15.831	-360.018	-309.390	84.520
900	34.571	52.878	31.472	19.265	-359.282	-303.103	73.603
1000	34.954	56.541	33.799	22.742	-358.561	-296.897	64.886
1100	35.268	59.888	36.022	26.253	-357.875	-290.778	57.771
1156	35.415	61.643	37.220	28.233	-357.501	-287.363	54.327
1156	35.415	61.643	37.220	28.233	-359.535	-287.363	54.327
1200	35.530	62.968	38.140	29.794	-359.155	-284.623	51.836
1300	35.750	65.821	40.161	33.358	-358.318	-278.447	46.811
1400	35.936	68.478	42.090	36.943	-357.510	-272.335	42.513
1500	36.091	70.962	43.933	40.544	-356.734	-266.276	38.796
1600	36.218	73.296	45.696	44.160	-355.998	-260.272	35.551
1700	36.321	75.495	47.385	47.787	-355.306	-254.309	32.693
1800	36.400	77.573	49.005	51.423	-354.674	-248.388	30.158
1900	36.458	79.543	50.561	55.066	-354.116	-242.498	27.893
1945	36.474	80.397	51.241	56.707	-353.895	-239.858	26.951
1945	36.474	80.397	51.241	56.707	-360.495	-239.858	26.951
2000	36.494	81.414	52.057	58.714	-360.447	-236.448	25.838

Phase changes: 473 K, α - β transition point of Ti_2O_3; $\Delta H° = 0.215$ kcal.mol.
1156 K, α - β transition point of Ti; $\Delta H° = 1.017$ kcal/mol.
1945 K, melting point of Ti; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-473 K:
$$Cp° = 14.971 + 40.290\times10^{-3}T - 3.621\times10^{5}T^{-2}$$
$$H°- H°_{298} = 14.971\times10^{-3}T + 20.145\times10^{-6}T^{2} + 3.621\times10^{2}T^{-1} - 7.469$$

473-2000 K:
$$Cp° = 34.421 + 1.400\times10^{-3}T - 9.404\times10^{5}T^{-2}$$
$$H°- H°_{298} = 34.421\times10^{-3}T + 0.700\times10^{-6}T^{2} + 9.404\times10^{2}T^{-1} - 13.326$$

Formation equations (kcal/mol):

298.15-473 K:
$$\Delta Hf° = -363.876 - 6.828\times10^{-3}T + 17.145\times10^{-6}T^{2} + 264.700T^{-1}$$
$$\Delta Gf° = -363.876 + 6.828\times10^{-3}T\ln T - 17.145\times10^{-6}T^{2} + 132.350T^{-1} + 35.649\times10^{-3}T$$

473-1156 K:
$$\Delta Hf° = -369.733 + 12.622\times10^{-3}T - 2.301\times10^{-6}T^{2} + 843.000T^{-1}$$
$$\Delta Gf° = -369.733 - 12.622\times10^{-3}T\ln T + 2.301\times10^{-6}T^{2} + 421.500T^{-1} + 157.336\times10^{-3}T$$

1156-1945 K:
$$\Delta Hf° = -377.807 + 17.422\times10^{-3}T - 2.947\times10^{-6}T^{2} + 2408.800T^{-1}$$
$$\Delta Gf° = -377.807 - 17.422\times10^{-3}T\ln T + 2.947\times10^{-6}T^{2} + 1204.400T^{-1} + 196.841\times10^{-3}T$$

1945-2000 K:
$$\Delta Hf° = -363.543 + 1.476\times10^{-3}T - 0.054\times10^{-6}T^{2} + 872.600T^{-1}$$
$$\Delta Gf° = -363.543 - 1.476\times10^{-3}T\ln T + 0.054\times10^{-6}T^{2} + 436.300T^{-1} + 74.576\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Wagman (238). Low-temperature heat capacities and entropy at 298 K from Paukov (183). High-temperature data based on Naylor (165).

Ti_3O_5(c)

Trititanium Pentoxide

[Formation: $3Ti(c,l) + 2.5O_2(g) = Ti_3O_5(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	37.000	30.920	30.920	0	-587.800	-553.944	406.047
300	37.180	31.149	30.920	.069	-587.797	-553.730	403.387
400	49.199	43.403	32.511	4.357	-587.131	-542.447	296.375
450	56.180	49.598	34.065	6.990	-586.362	-536.909	260.755
450	46.384	54.709	34.065	9.290	-584.062	-536.909	260.755
500	46.148	59.582	36.376	11.603	-583.642	-531.692	232.399
600	46.126	67.985	40.965	16.212	-582.913	-521.372	189.907
700	46.598	75.126	45.349	20.844	-582.292	-511.149	159.586
800	47.450	81.400	49.470	25.544	-581.727	-501.030	136.873
900	48.576	87.052	53.338	30.343	-581.176	-490.974	119.223
1000	49.879	92.236	56.971	35.265	-580.596	-480.977	105.116
1100	51.275	97.055	60.399	40.322	-579.985	-471.063	93.590
1156	52.067	99.620	62.236	43.216	-579.620	-465.516	88.008
1156	52.067	99.620	62.236	43.216	-582.670	-465.516	88.008
1200	52.689	101.577	63.643	45.521	-582.232	-461.065	83.970
1300	54.056	105.849	66.727	50.858	-581.198	-451.011	75.821
1400	55.321	109.902	69.668	56.328	-580.110	-441.038	68.848
1500	56.440	113.758	72.479	61.918	-578.976	-431.141	62.816
1600	57.379	117.431	75.175	67.610	-577.822	-421.325	57.550
1700	58.115	120.933	77.764	73.387	-576.668	-411.576	52.911
1800	58.632	124.271	80.257	79.226	-575.557	-401.900	48.797
1900	58.929	127.450	82.657	85.106	-574.528	-392.279	45.122
1945	58.966	128.830	83.710	87.759	-574.106	-387.971	43.594
1945	58.966	128.830	83.710	87.759	-584.006	-387.971	43.594
2000	59.012	130.475	84.973	91.005	-583.821	-382.429	41.789

Phase changes: 450 K, α - β transition point of Ti_3O_5; $\Delta H° = 2.300$ kcal/mol.
1156 K, α - β transition point of Ti; $\Delta H° = 1.017$ kcal/mol.
1945 K, melting point of Ti; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-450 K:
$$Cp° = -21.447 + 162.886\times10^{-3}T + 8.785\times10^{5}T^{-2}$$
$$H°- H°_{298} = -21.447\times10^{-3}T + 81.443\times10^{-6}T^{2} - 8.785\times10^{2}T^{-1} + 2.101$$

450-2000 K:
$$Cp° = 36.005 + 12.938\times10^{-3}T + 9.227\times10^{5}T^{-2}$$
$$H°- H°_{298} = 36.005\times10^{-3}T + 6.469\times10^{-6}T^{2} - 9.227\times10^{2}T^{-1} - 6.172$$

Formation equations (kcal/mol):

298.15-450 K:
$$\Delta Hf° = -574.472 - 55.953\times10^{-3}T + 76.816\times10^{-6}T^{2} - 1035.900T^{-1}$$
$$\Delta Gf° = -574.472 + 55.953\times10^{-3}T\ln T - 76.816\times10^{-6}T^{2} - 517.950T^{-1} - 221.219\times10^{-3}T$$

450-1156 K:
$$\Delta Hf° = -582.745 + 1.499\times10^{-3}T + 1.842\times10^{-6}T^{2} - 1080.100T^{-1}$$
$$\Delta Gf° = -582.745 - 1.499\times10^{-3}T\ln T - 1.842\times10^{-6}T^{2} - 540.050T^{-1} + 114.525\times10^{-3}T$$

1156-1945 K:
$$\Delta Hf° = -594.856 + 8.699\times10^{-3}T + 0.874\times10^{-6}T^{2} + 1268.600T^{-1}$$
$$\Delta Gf° = -594.856 - 8.699\times10^{-3}T\ln T - 0.874\times10^{-6}T^{2} + 634.300T^{-1} + 173.782\times10^{-3}T$$

1945-2000 K:
$$\Delta Hf° = -573.459 - 15.220\times10^{-3}T + 5.212\times10^{-6}T^{2} - 1035.700T^{-1}$$
$$\Delta Gf° = -573.459 + 15.220\times10^{-3}T\ln T - 5.212\times10^{-6}T^{2} - 517.850T^{-1} - 9.616\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Wagman (238). Low-temperature heat capacities and entropy at 298 K from Shomate (197). High-temperature data based on Naylor (165) and Slyusar (204).

$Ti_4O_7(c)$

Tetratitanium Heptoxide

[Formation: $4Ti(c,l) + 3.5O_2(g) = Ti_4O_7(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	51.560	47.000	47.000	0	-813.000	-767.145	562.325
300	51.706	47.319	47.000	.096	-812.993	-766.856	558.647
400	57.345	63.046	49.106	5.576	-812.463	-751.547	410.621
500	60.772	76.235	53.249	11.493	-811.676	-736.412	321.881
600	63.271	87.546	58.046	17.700	-810.768	-721.443	262.782
700	65.294	97.456	62.983	24.131	-809.815	-706.607	220.610
800	67.028	106.290	67.854	30.749	-808.842	-691.938	189.026
900	68.564	114.275	72.575	37.530	-807.863	-677.379	164.488
1000	69.948	121.572	77.115	44.457	-806.862	-662.929	144.881
1100	71.208	128.299	81.466	51.516	-805.872	-648.609	128.865
1156	71.854	131.851	83.822	55.522	-805.315	-640.603	121.109
1156	71.854	131.851	83.822	55.522	-809.383	-640.603	121.109
1200	72.361	134.545	85.632	58.695	-808.760	-634.190	115.500
1300	73.415	140.379	89.621	65.985	-807.351	-619.700	104.180
1400	74.378	145.855	93.444	73.375	-805.948	-605.319	94.493
1500	75.254	151.017	97.112	80.857	-804.552	-591.035	86.113
1600	76.047	155.900	100.636	88.423	-803.183	-576.849	78.793
1700	76.758	160.532	104.024	96.064	-801.853	-562.739	72.344
1800	77.390	164.938	107.287	103.772	-800.597	-548.714	66.622
1900	77.944	169.137	110.432	111.539	-799.447	-534.749	61.509
1945	78.158	170.964	111.812	115.051	-798.977	-528.490	59.383
1945	78.158	170.964	111.812	115.051	-812.177	-528.490	59.383
2000	78.420	173.147	113.468	119.358	-812.035	-520.471	56.874

Phase changes: 1156 K, α - β transition point of Ti; $\Delta H° = 1.017$ kcal/mol.
1945 K, melting point of Ti; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 59.609 + 10.824\times10^{-3}T - 10.024\times10^{5}T^{-2}$

$H°- H°_{298} = 59.609\times10^{-3}T + 5.412\times10^{-6}T^{2} + 10.024\times10^{2}T^{-1} - 21.616$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -819.254 + 12.396\times10^{-3}T - 0.841\times10^{-6}T^{2} + 785.000T^{-1}$

$\Delta Gf° = -819.254 - 12.396\times10^{-3}T\ln T + 0.841\times10^{-6}T^{2} + 392.500T^{-1} + 240.735\times10^{-3}T$

1156-1945 K: $\Delta Hf° = -835.402 + 21.996\times10^{-3}T - 2.132\times10^{-6}T^{2} + 3916.600T^{-1}$

$\Delta Gf° = -835.402 - 21.996\times10^{-3}T\ln T + 2.132\times10^{-6}T^{2} + 1958.300T^{-1} + 319.745\times10^{-3}T$

1945-2000 K: $\Delta Hf° = -806.873 - 9.896\times10^{-3}T + 3.651\times10^{-6}T^{2} + 844.200T^{-1}$

$\Delta Gf° = -806.873 + 9.896\times10^{-3}T\ln T - 3.651\times10^{-6}T^{2} + 422.100T^{-1} + 75.214\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Vasil'eva (233). Low-temperature heat capacities and entropy at 298 K from Beresovskii (18). High-temperature data based on Slyusar (204).

Tl(c,l,g)

Thallium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.290	15.340	15.340	0
300	6.300	15.380	15.340	.012
400	6.560	17.220	15.587	.653
500	7.030	18.730	16.070	1.330
507	7.090	18.830	16.110	1.380
507	7.650	19.010	16.110	1.470
577	7.810	20.010	16.522	2.011
577	7.100	21.720	16.522	3.001
600	7.100	22.000	16.727	3.164
700	7.100	23.100	17.566	3.874
800	7.100	24.040	18.310	4.584
900*	7.100	24.880	18.998	5.294
1000	7.100	25.630	19.626	6.004
1100	7.100	26.310	20.206	6.714
1200	7.100	26.920	20.733	7.424
1300	7.100	27.490	21.233	8.134
1400	7.100	28.020	21.703	8.844
1500	7.100	28.510	22.141	9.554
1600	7.100	28.970	22.555	10.264
1700	7.100	29.400	22.945	10.974
1746	7.100	29.590	23.118	11.301
1746	5.234	52.050	23.118	50.516
1800	5.270	52.213	23.992	50.798
1900	5.343	52.500	25.485	51.329
2000	5.420	52.776	26.843	51.866

*Data 900 K to 1746 K extrapolated.

Phase changes: 507 K, $\alpha - \beta$ transition point of Tl; ΔH° = 0.090 kcal/mol.
577 K, melting point of Tl; ΔH° = 0.990 kcal/mol.
1746 K, boiling point of Tl; ΔH° = 39.215 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-507 K: $Cp^\circ = 4.026 + 5.500\times10^{-3}T + 0.554\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.026\times10^{-3}T + 2.750\times10^{-6}T^2 - 0.554\times10^{2}T^{-1} - 1.259$

507-577 K: $Cp^\circ = 6.491 + 2.286\times10^{-3}T$

$H^\circ - H^\circ_{298} = 6.491\times10^{-3}T + 1.143\times10^{-6}T^2 - 2.115$

577-1746 K: $Cp^\circ = 7.100$

$H^\circ - H^\circ_{298} = 7.100\times10^{-3}T - 1.096$

1746-2000 K: $Cp^\circ = 5.163 + 0.080\times10^{-3}T$

$H^\circ - H^\circ_{298} = 5.163\times10^{-3}T + 0.040\times10^{-6}T^2 + 41.379$

Source: Data from Hultgren (99) who extrapolated 900 K to 1746 K assuming constant heat capacity.

Tl(g)

Thallium (ideal monatomic gas)

[Formation: Tl(c,l,g) = Tl(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	43.226	43.226	0	43.250	34.936	-25.608
300	4.968	43.256	43.226	.009	43.247	34.884	-25.413
400	4.968	44.685	43.420	.506	43.103	32.117	-17.548
500	4.968	45.794	43.788	1.003	42.923	29.391	-12.847
507	4.968	45.863	43.816	1.038	42.908	29.202	-12.588
507	4.968	45.863	43.816	1.038	42.818	29.202	-12.588
577	4.968	46.506	44.104	1.386	42.625	27.335	-10.354
577	4.968	46.506	44.104	1.386	41.635	27.335	-10.354
600	4.968	46.700	44.200	1.500	41.586	26.766	-9.749
700	4.968	47.466	44.615	1.996	41.372	24.316	-7.592
800	4.969	48.129	45.013	2.493	41.159	21.888	-5.979
900	4.970	48.714	45.392	2.990	40.946	19.495	-4.734
1000	4.975	49.238	45.751	3.487	40.733	17.125	-3.743
1100	4.983	49.713	46.090	3.985	40.521	14.778	-2.936
1200	4.998	50.147	46.410	4.484	40.310	12.438	-2.265
1300	5.021	50.548	46.713	4.985	40.101	10.126	-1.702
1400	5.053	50.921	47.000	5.489	39.895	7.834	-1.223
1500	5.094	51.271	47.274	5.996	39.692	5.550	-.809
1600	5.144	51.601	47.534	6.508	39.494	3.284	-.449
1700	5.203	51.915	47.783	7.025	39.301	1.026	-.132
1746	5.234	52.054	47.893	7.265	39.215	0	0
1746	5.234	52.054	47.893	7.265	0	0	0
1800	5.270	52.213	48.019	7.549	0	0	0
1900	5.343	52.500	48.248	8.079	0	0	0
2000	5.420	52.776	48.468	8.617	0	0	0

Phase changes: 507 K, α - β transition point of Tl; ΔH° = 0.090 kcal/mol.
577 K, melting point of Tl; ΔH° = 0.990 kcal/mol.
1746 boiling point of Tl; ΔH° = 39.215

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.810 + 0.198\times10^{-3}T + 0.088\times10^{5}T^{-2}$

$H°- H°_{298} = 4.810\times10^{-3}T + 0.099\times10^{-6}T^{2} - 0.088\times10^{2}T^{-1} - 1.413$

Formation equations (kcal/mol):

298.15-507 K: $\Delta Hf° = 43.096 + 0.784\times10^{-3}T - 2.651\times10^{-6}T^{2} + 46.600T^{-1}$

$\Delta Gf° = 43.096 - 0.784\times10^{-3}T\ln T + 2.651\times10^{-6}T^{2} + 23.300T^{-1} - 23.954\times10^{-3}T$

507-577 K: $\Delta Hf° = 43.952 - 1.681\times10^{-3}T - 1.044\times10^{-6}T^{2} - 8.800T^{-1}$

$\Delta Gf° = 43.952 + 1.681\times10^{-3}T\ln T + 1.044\times10^{-6}T^{2} - 4.400T^{-1} - 40.073\times10^{-3}T$

577-1746 K: $\Delta Hf° = 42.932 - 2.290\times10^{-3}T + 0.099\times10^{-6}T^{2} - 8.800T^{-1}$

$\Delta Gf° = 42.932 + 2.290\times10^{-3}T\ln T - 0.099\times10^{-6}T^{2} - 4.400T^{-1} - 41.519\times10^{-3}T$

1746-2000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Sources: Enthalpy of formation at 298 K from Hultgren (99). All other data from Hilsenrath (94).

$Tl_2O(c,l)$

Dithallium Oxide

[Formation: $2Tl(c,l) + 0.5O_2(g) = Tl_2O(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	18.850	34.700	34.700	0	-40.400	-34.293	25.137
300	18.867	34.817	34.700	.035	-40.396	-34.255	24.955
400	19.620	40.353	35.451	1.961	-40.107	-32.254	17.622
500	20.230	44.799	36.891	3.954	-39.833	-30.322	13.254
507	20.269	45.081	37.002	4.096	-39.817	-30.188	13.013
507	20.269	45.081	37.002	4.096	-39.997	-30.188	13.013
577	20.657	47.727	38.144	5.529	-39.909	-28.838	10.923
577	20.657	47.727	38.144	5.529	-41.889	-28.838	10.923
600	20.785	48.537	38.527	6.006	-41.826	-28.320	10.315
700	21.314	51.781	40.194	8.111	-41.531	-26.084	8.144
800	21.829	54.660	41.825	10.268	-41.193	-23.912	6.533
852	22.094	56.043	42.651	11.410	-41.000	-22.789	5.846
852	26.700	64.506	42.651	18.620	-33.790	-22.789	5.846
900	26.700	65.969	43.856	19.902	-33.386	-22.180	5.386
1000	26.700	68.782	46.210	22.572	-32.549	-20.976	4.584

*Heat capacity at 298 K estimated.

Phase changes: 507 K, α - β transition point of Tl; $\Delta H° = 0.090$ kcal/mol.
577 K, melting point of Tl; $\Delta H° = 0.990$ kcal/mol.
852 K, melting point of Tl_2O; $\Delta H° = 7.210$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-852 K: $Cp° = 18.025 + 4.858\times10^{-3}T - 0.555\times10^{5}T^{-2}$

$H°- H°_{298} = 18.025\times10^{-3}T + 2.429\times10^{-6}T^{2} + 0.555\times10^{2}T^{-1} - 5.776$

852-1000 K: $Cp° = 26.700$

$H°- H°_{298} = 26.700\times10^{-3}T - 4.128$

Formation equations (kcal/mol):

298.15-507 K: $\Delta Hf° = -42.482 + 6.358\times10^{-3}T - 3.322\times10^{-6}T^{2} + 143.700T^{-1}$

$\Delta Gf° = -42.482 - 6.358\times10^{-3}T\ln T + 3.322\times10^{-6}T^{2} + 71.850T^{-1} + 61.893\times10^{-3}T$

507-577 K: $\Delta Hf° = -40.770 + 1.428\times10^{-3}T - 0.108\times10^{-6}T^{2} + 32.900T^{-1}$

$\Delta Gf° = -40.770 - 1.428\times10^{-3}T\ln T + 0.108\times10^{-6}T^{2} + 16.450T^{-1} + 29.655\times10^{-3}T$

577-852 K: $\Delta Hf° = -42.809 + 0.210\times10^{-3}T + 2.178\times10^{-6}T^{2} + 32.900T^{-1}$

$\Delta Gf° = -42.809 - 0.210\times10^{-3}T\ln T - 2.178\times10^{-6}T^{2} + 16.450T^{-1} + 26.763\times10^{-3}T$

852-1000 K: $\Delta Hf° = -41.161 + 8.885\times10^{-3}T - 0.251\times10^{-6}T^{2} - 22.600T^{-1}$

$\Delta Gf° = -41.161 - 8.885\times10^{-3}T\ln T + 0.251\times10^{-6}T^{2} - 11.300T^{-1} + 81.333\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Cubicciotti (45,46). High-temperature data based on Cubicciotti (47). Heat capacity at 298 K estimated.

$Tl_2O(g)$

Dithallium Oxide (ideal gas)

[Formation: $2Tl(c,l) + 0.5O_2(g) = Tl_2O(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.470	75.850	75.850	0	1.500	-4.662	3.417
300	12.480	75.930	75.853	.023	1.492	-4.701	3.425
400	13.000	79.600	76.355	1.298	1.131	-6.715	3.669
500	13.280	82.530	77.304	2.613	.726	-8.629	3.772
507	13.293	82.715	77.377	2.706	.693	-8.758	3.775
507	13.293	82.715	77.377	2.706	.513	-8.758	3.775
577	13.419	84.445	78.133	3.642	.103	-10.012	3.792
577	13.419	84.445	78.133	3.642	-1.877	-10.012	3.792
600	13.460	84.970	78.385	3.951	-1.982	-10.334	3.764
700	13.580	87.050	79.474	5.303	-2.438	-11.680	3.647
800	13.640	88.870	80.540	6.664	-2.896	-12.985	3.547
900	13.700	90.480	81.557	8.031	-3.357	-14.211	3.451
1000	13.740	91.930	82.527	9.403	-3.818	-15.393	3.364

Phase changes: 507 K, α - β transition point of Tl; $\Delta H° = 0.090$ kcal/mol.
577 K, melting point of Tl; $\Delta H° = 0.990$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 13.292 + 0.648\times10^{-3}T - 0.903\times10^{5}T^{-2}$

$H°- H°_{298} = 13.292\times10^{-3}T + 0.324\times10^{-6}T^{2} + 0.903\times10^{2}T^{-1} - 4.295$

Formation equations (kcal/mol):

298.15-507 K: $\Delta Hf° = 0.899 + 1.625\times10^{-3}T - 5.428\times10^{-6}T^{2} + 178.500T^{-1}$

$\Delta Gf° = 0.899 - 1.625\times10^{-3}T\ln T + 5.428\times10^{-6}T^{2} + 89.250T^{-1} - 12.016\times10^{-3}T$

507-577 K: $\Delta Hf° = 2.611 - 3.305\times10^{-3}T - 2.214\times10^{-6}T^{2} + 67.700T^{-1}$

$\Delta Gf° = 2.611 + 3.305\times10^{-3}T\ln T + 2.214\times10^{-6}T^{2} + 33.850T^{-1} - 44.254\times10^{-3}T$

577-1000 K: $\Delta Hf° = 0.573 - 4.523\times10^{-3}T + 0.072\times10^{-6}T^{2} + 67.700T^{-1}$

$\Delta Gf° = 0.573 + 4.523\times10^{-3}T\ln T - 0.072\times10^{-6}T^{2} + 33.850T^{-1} - 47.147\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Cubicciotti (45). All other data based on Cubicciotti (46).

$Tl_2O_3(c)$

Dithallium Trioxide, Thallium Sesquioxide

[Formation: $2Tl(c,l) + 1.5O_2(g) = Tl_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	25.200	38.000	38.000	0	-94.300	-74.566	54.658
300	25.296	38.156	38.000	.047	-94.297	-74.443	54.231
400	28.653	45.959	39.042	2.767	-93.924	-67.877	37.086
500	30.242	52.542	41.102	5.720	-93.421	-61.421	26.847
507	30.304	52.963	41.263	5.932	-93.387	-60.972	26.282
507	30.304	52.963	41.263	5.932	-93.567	-60.972	26.282
577	30.926	56.929	42.927	8.079	-93.292	-56.490	21.396
577	30.926	56.929	42.927	8.079	-95.272	-56.490	21.396
600	31.130	58.142	43.487	8.793	-95.149	-54.946	20.014
700	31.687	62.985	45.935	11.935	-94.594	-48.282	15.074
800	32.067	67.243	48.338	15.124	-94.022	-41.720	11.397
900	32.344	71.036	50.653	18.345	-93.442	-35.209	8.550
1000	32.557	74.456	52.865	21.591	-92.856	-28.767	6.287

*Heat capacity at 298 K estimated.

Phase changes: 507 K, α - β transition point of Tl; $\Delta H°$ = 0.090 kcal/mol.
577 K, melting point of Tl; $\Delta H°$ = 0.990 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 32.675 + 0.564\times10^{-3}T - 6.794\times10^{5}T^{-2}$

$H°- H°_{298} = 32.675\times10^{-3}T + 0.282\times10^{-6}T^{2} + 6.794\times10^{2}T^{-1} - 12.046$

Formation equations (kcal/mol):

298.15-507 K: $\Delta Hf° = -100.300 + 13.778\times10^{-3}T - 5.972\times10^{-6}T^{2} + 722.400T^{-1}$

$\Delta Gf° = -100.300 - 13.778\times10^{-3}T\ln T + 5.972\times10^{-6}T^{2} + 361.200T^{-1} + 158.969\times10^{-3}T$

507-577 K: $\Delta Hf° = -98.588 + 8.848\times10^{-3}T - 2.758\times10^{-6}T^{2} + 611.600T^{-1}$

$\Delta Gf° = -98.588 - 8.848\times10^{-3}T\ln T + 2.758\times10^{-6}T^{2} + 305.800T^{-1} + 126.731\times10^{-3}T$

577-1000 K: $\Delta Hf° = -100.626 + 7.630\times10^{-3}T - 0.472\times10^{-6}T^{2} + 611.600T^{-1}$

$\Delta Gf° = -100.626 - 7.630\times10^{-3}T\ln T + 0.472\times10^{-6}T^{2} + 305.800T^{-1} + 123.839\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Cubicciotti (45,46). Heat capacity at 298 K estimated. High-temperature data based on Cubicciotti (47) and Mills (157).

Tm(c,l)

Thulium

T, K	cal/mol•K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.460	17.690	17.690	0
300	6.460	17.730	17.690	.012
400	6.490	19.590	17.940	.660
500	6.510	21.040	18.420	1.310
600	6.590	22.230	18.958	1.963
700	6.760	23.260	19.504	2.629
800	7.080	24.180	20.029	3.321
900	7.330	25.030	20.540	4.041
1000	7.520	25.820	21.034	4.786
1100	7.710	26.540	21.496	5.548
1200	7.890	27.220	21.947	6.328
1300	8.080	27.860	22.378	7.126
1400	8.250	28.470	22.797	7.942
1500	8.430	29.040	23.189	8.776
1600	8.600	29.590	23.573	9.628
1700	8.770	30.120	23.945	10.497
1800	8.930	30.620	24.297	11.382
1818	8.960	30.710	24.364	11.543
1818	9.890	32.930	24.364	15.568
1900	9.890	33.360	24.739	16.379
2000	9.890	33.870	25.177	17.386

Phase changes: 1818 K, melting point of Tm; ΔH° = 4.025 kcal/mol.
2220 K, boiling point of Tm; ΔH° = 45.6 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1818 K: $Cp^\circ = 5.321 + 2.068\times10^{-3}T + 0.464\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.321\times10^{-3}T + 1.034\times10^{-6}T^2 - 0.464\times10^{2}T^{-1} - 1.523$

1818-2000 K: $Cp^\circ = 9.890$

$H^\circ - H^\circ_{298} = 9.890\times10^{-3}T - 2.412$

Source: Data from Hultgren (99).

Tm(g)

Thulium (ideal monatomic gas)

[Formation: Tm(c,1) = Tm(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH_f°	ΔG_f°	
298.15	4.968	45.412	45.412	0	55.500	47.235	-34.624
300	4.968	45.443	45.413	.009	55.497	47.183	-34.372
400	4.968	46.872	45.607	.506	55.346	44.433	-24.277
500	4.968	47.981	45.975	1.003	55.193	41.722	-18.237
600	4.968	48.886	46.386	1.500	55.037	39.043	-14.221
700	4.968	49.652	46.801	1.996	54.867	36.393	-11.362
800	4.968	50.316	47.200	2.493	54.672	33.763	-9.224
900	4.968	50.901	47.579	2.990	54.449	31.165	-7.568
1000	4.969	51.424	47.937	3.487	54.201	28.597	-6.250
1100	4.970	51.898	48.276	3.984	53.936	26.042	-5.174
1200	4.973	52.330	48.596	4.481	53.653	23.521	-4.284
1300	4.977	52.729	48.900	4.978	53.352	21.022	-3.534
1400	4.984	53.098	49.187	5.476	53.034	18.555	-2.896
1500	4.993	53.442	49.459	5.975	52.699	16.096	-2.345
1600	5.007	53.764	49.717	6.475	52.347	13.669	-1.867
1700	5.024	54.068	49.964	6.977	51.980	11.268	-1.449
1800	5.047	54.356	50.200	7.480	51.598	8.873	-1.077
1818	5.052	54.406	50.242	7.571	51.528	8.454	-1.016
1818	5.052	54.406	50.242	7.571	47.503	8.454	-1.016
1900	5.076	54.630	50.427	7.986	47.107	6.694	-.770
2000	5.112	54.891	50.643	8.496	46.610	4.568	-.499

Phase change: 1818 K, melting point of Tm; ΔH° = 4.025 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 4.932 + 0.046\times10^{-3}T + 0.020\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.932\times10^{-3}T + 0.023\times10^{-6}T^2 - 0.020\times10^{2}T^{-1} - 1.466$

Formation equations (kcal/mol):

298.15-1818 K: $\Delta H_f^\circ = 55.557 - 0.389\times10^{-3}T - 1.011\times10^{-6}T^2 + 44.400T^{-1}$

$\Delta G_f^\circ = 55.557 + 0.389\times10^{-3}T\ln T + 1.011\times10^{-6}T^2 + 22.200T^{-1} - 30.680\times10^{-3}T$

1818-2000 K: $\Delta H_f^\circ = 56.446 - 4.958\times10^{-3}T + 0.023\times10^{-6}T^2 - 2.000T^{-1}$

$\Delta G_f^\circ = 56.446 + 4.958\times10^{-3}T\ln T - 0.023\times10^{-6}T^2 - 1.000T^{-1} - 63.576\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). All other data from Feber (59).

$Tm_2O_3(c)$

Dithulium Trioxide, Thulium Sesquioxide

[Formation: $2Tm(c,l) + 1.5O_2(g) = Tm_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	27.900	33.400	33.400	0	-451.400	-428.893	314.383
300	27.941	33.573	33.400	.052	-451.391	-428.753	312.343
400	29.355	41.832	34.517	2.926	-450.879	-421.285	230.177
500	30.030	48.463	36.665	5.899	-450.302	-413.953	180.936
600	30.434	53.976	39.104	8.923	-449.716	-406.739	148.153
700	30.724	58.690	41.573	11.982	-449.156	-399.615	124.764
800	30.962	62.809	43.976	15.066	-448.653	-392.581	107.247
900	31.173	66.468	46.276	18.173	-448.207	-385.594	93.634
1000	31.368	69.762	48.462	21.300	-447.811	-378.648	82.752
1100	31.549	72.761	50.537	24.446	-447.448	-371.763	73.862
1200	31.713	75.513	52.505	27.610	-447.116	-364.893	66.455
1300	31.857	78.057	54.374	30.788	-446.818	-358.050	60.193
1400	31.975	80.423	56.152	33.980	-446.553	-351.218	54.827
1500	32.061	82.632	57.844	37.182	-446.324	-344.433	50.183
1600	32.109	84.703	59.459	40.391	-446.135	-337.646	46.120
1680	32.114	86.269	60.698	42.960	-446.011	-332.213	43.217
1680	32.000	86.454	60.698	43.270	-445.701	-332.213	43.217
1700	32.000	86.833	61.004	43.910	-445.677	-330.862	42.535
1800	32.000	88.662	62.490	47.110	-445.579	-324.131	39.354
1818	32.000	88.980	62.750	47.686	-445.566	-322.902	38.817
1818	32.000	88.980	62.750	47.686	-453.616	-322.902	38.817
1900	32.000	90.392	63.913	50.310	-453.714	-317.018	36.465
2000	32.000	92.033	65.278	53.510	-453.876	-309.844	33.858

Phase changes: 1680 K, α - β transition point of Tm_2O_3; $\Delta H° = 0.310$ kcal/mol.
1818 K, melting point of Tm; $\Delta H° = 4.025$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1680 K: $Cp° = 30.561 + 1.068\times10^{-3}T - 2.648\times10^{5}T^{-2}$

$H°- H°_{298} = 30.561\times10^{-3}T + 0.534\times10^{-6}T^2 + 2.648\times10^{2}T^{-1} - 10.047$

1680-2000 K: $Cp° = 32.000$

$H°- H°_{298} = 32.000\times10^{-3}T - 10.490$

Formation equations (kcal/mol):

298.15-1680 K: $\Delta Hf° = -454.874 + 9.074\times10^{-3}T - 2.288\times10^{-6}T^2 + 289.800T^{-1}$

$\Delta Gf° = -454.874 - 9.074\times10^{-3}T\ln T + 2.288\times10^{-6}T^2 + 144.900T^{-1} + 136.527\times10^{-3}T$

1680-1818 K: $\Delta Hf° = -455.317 + 10.513\times10^{-3}T - 2.822\times10^{-6}T^2 + 25.000T^{-1}$

$\Delta Gf° = -455.317 - 10.513\times10^{-3}T\ln T + 2.822\times10^{-6}T^2 + 12.500T^{-1} + 146.627\times10^{-3}T$

1818-2000 K: $\Delta Hf° = -453.538 + 1.375\times10^{-3}T - 0.754\times10^{-6}T^2 - 67.800T^{-1}$

$\Delta Gf° = -453.538 - 1.375\times10^{-3}T\ln T + 0.754\times10^{-6}T^2 - 33.900T^{-1} + 80.837\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). Low-temperature heat capacities and entropy at 298 K from Justice (112). High-temperature data based on Pankratz (178).

U(c,1)

Uranium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.612	12.000	12.000	0
300	6.621	12.041	12.001	.012
400	7.095	14.009	12.264	.698
500	7.648	15.650	12.782	1.434
600	8.308	17.101	13.383	2.231
700	9.087	18.439	14.012	3.099
800	9.988	19.709	14.644	4.052
900	11.014	20.944	15.276	5.101
942	11.481	21.457	15.540	5.574
942	10.260	22.165	15.540	6.241
1000	10.260	22.778	15.942	6.836
1049	10.260	23.269	16.274	7.338
1049	9.150	24.353	16.274	8.475
1100	9.150	24.787	16.658	8.942
1200	9.150	25.583	17.369	9.857
1300	9.150	26.315	18.029	10.772
1400	9.150	26.994	18.646	11.687
1408	9.150	27.046	18.694	11.760
1408	11.630	28.598	18.694	13.945
1500	11.630	29.334	19.324	15.015
1600	11.630	30.084	19.973	16.178
1700*	11.630	30.789	20.588	17.341
1800	11.630	31.454	21.174	18.504
1900	11.630	32.083	21.732	19.667
2000	11.630	32.679	22.264	20.830
2100	11.630	33.247	22.774	21.993
2200	11.630	33.788	23.263	23.156
2300	11.630	34.305	23.732	24.319
2400	11.630	34.800	24.182	25.482
2500	11.630	35.275	24.617	26.645
2600	11.630	35.731	25.036	27.808
2700	11.630	36.170	25.440	28.971
2800	11.630	36.593	25.831	30.134
2900	11.630	37.001	26.209	31.297
3000	11.630	37.395	26.575	32.460
3100	11.630	37.776	26.930	33.623
3200	11.630	38.146	27.275	34.786
3300	11.630	38.503	27.609	35.949
3400	11.630	38.851	27.936	37.112
3500	11.630	39.188	28.252	38.275

*Data above 1600 K extrapolated.

U(c,l) - Continued

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-942 K:

$$Cp^\circ = 3.110 + 8.444\times10^{-3}T + 0.875\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 3.110\times10^{-3}T + 4.222\times10^{-6}T^2 - 0.875\times10^{2}T^{-1} - 1.009$$

942-1049 K:

$$Cp^\circ = 10.255$$

$$H^\circ - H^\circ_{298} = 10.255\times10^{-3}T - 3.419$$

1049-1408 K:

$$Cp^\circ = 9.150$$

$$H^\circ - H^\circ_{298} = 9.150\times10^{-3}T - 1.123$$

1408-3500 K:

$$Cp^\circ = 11.630$$

$$H^\circ - H^\circ_{298} = 11.630\times10^{-3}T - 2.430$$

Source: Data from Oetting (167) who extrapolated above 1600 K by assuming constant heat capacity.

U(g)

Uranium (ideal monatomic gas)

[Formation: U(c,1) = U(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.663	47.724	47.724	0	127.000	116.349	-85.285
300	5.666	47.759	47.726	.010	126.998	116.283	-84.711
400	5.724	49.402	47.947	.582	126.884	112.727	-61.590
500	5.665	50.674	48.372	1.151	126.717	109.205	-47.733
600	5.593	51.700	48.843	1.714	126.483	105.724	-38.509
700	5.559	52.559	49.315	2.271	126.172	102.288	-31.935
800	5.580	53.302	49.767	2.828	125.776	98.902	-27.018
900	5.661	53.963	50.197	3.389	125.288	95.571	-23.207
942	5.718	54.222	50.371	3.628	125.054	94.189	-21.852
942	5.718	54.222	50.371	3.628	124.387	94.189	-21.852
1000	5.796	54.566	50.604	3.962	124.126	92.338	-20.180
1049	5.885	54.845	50.796	4.248	123.910	90.787	-18.914
1049	5.885	54.845	50.796	4.248	122.773	90.787	-18.914
1100	5.978	55.127	50.991	4.550	122.608	89.234	-17.729
1200	6.199	55.656	51.357	5.159	122.302	86.214	-15.702
1300	6.453	56.162	51.707	5.791	122.019	83.218	-13.990
1400	6.731	56.651	52.044	6.450	121.763	80.243	-12.526
1408	6.755	56.689	52.070	6.504	121.744	80.006	-12.418
1408	6.755	56.689	52.070	6.504	119.559	80.006	-12.418
1500	7.028	57.125	52.366	7.138	119.123	77.437	-11.282
1600	7.340	57.588	52.678	7.856	118.678	74.672	-10.200
1700	7.663	58.043	52.981	8.606	118.265	71.933	-9.248
1800	7.992	58.490	53.274	9.389	117.885	69.220	-8.404
1900	8.325	58.931	53.560	10.205	117.538	66.527	-7.652
2000	8.659	59.367	53.840	11.054	117.224	63.848	-6.977
2100	8.992	59.797	54.113	11.937	116.944	61.189	-6.368
2200	9.321	60.223	54.381	12.852	116.696	58.539	-5.815
2300	9.643	60.645	54.645	13.801	116.482	55.900	-5.312
2400	9.957	61.062	54.903	14.781	116.299	53.270	-4.851
2500	10.259	61.475	55.158	15.792	116.147	50.647	-4.428

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 4.158 + 1.948\times10^{-3}T + 0.822\times10^{5}T^{-2}$

$H°- H°_{298} = 4.158\times10^{-3}T + 0.974\times10^{-6}T^{2} - 0.822\times10^{2}T^{-1} - 1.051$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf° = 126.958 + 1.048\times10^{-3}T - 3.248\times10^{-6}T^{2} + 5.300T^{-1}$

$\Delta Gf° = 126.958 - 1.048\times10^{-3}T\ln T + 3.248\times10^{-6}T^{2} + 2.650T^{-1} - 30.612\times10^{-3}T$

942-1049 K: $\Delta Hf° = 129.369 - 6.097\times10^{-3}T + 0.974\times10^{-6}T^{2} - 82.200T^{-1}$

$\Delta Gf° = 129.369 + 6.097\times10^{-3}T\ln T - 0.974\times10^{-6}T^{2} - 41.100T^{-1} - 78.073\times10^{-3}T$

1049-1408 K: $\Delta Hf° = 127.072 - 4.992\times10^{-3}T + 0.974\times10^{-6}T^{2} - 82.200T^{-1}$

$\Delta Gf° = 127.072 + 4.992\times10^{-3}T\ln T - 0.974\times10^{-6}T^{2} - 41.100T^{-1} - 68.198\times10^{-3}T$

1408-2500 K: $\Delta Hf° = 128.379 - 7.472\times10^{-3}T + 0.974\times10^{-6}T^{2} - 82.200T^{-1}$

$\Delta Gf° = 128.379 + 7.472\times10^{-3}T\ln T - 0.974\times10^{-6}T^{2} - 41.100T^{-1} - 87.106\times10^{-3}T$

Source: Data from Oetting (167).

$UO_2(c)$

Uranium Dioxide

[Formation: $U(c,l) + O_2(g) = UO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	15.200	18.410	18.410	0	-259.200	-246.500	180.687
300	15.242	18.504	18.411	.028	-259.197	-246.421	179.515
400	17.081	23.184	19.037	1.659	-258.962	-242.196	132.328
500	18.180	27.121	20.271	3.425	-258.663	-238.038	104.045
600	18.976	30.509	21.701	5.285	-258.355	-233.942	85.212
700	19.571	33.481	23.175	7.214	-258.072	-229.894	71.775
800	20.009	36.125	24.632	9.194	-257.843	-225.888	61.709
900	20.322	38.501	26.044	11.211	-257.689	-221.903	53.885
942	20.412	39.430	26.621	12.066	-257.653	-220.235	51.095
942	20.412	39.430	26.621	12.066	-258.320	-220.235	51.095
1000	20.537	40.654	27.399	13.255	-258.207	-217.893	47.620
1049	20.609	41.638	28.041	14.263	-258.111	-215.919	44.984
1049	20.609	41.638	28.041	14.263	-259.248	-215.919	44.984
1100	20.683	42.619	28.694	15.317	-259.090	-213.816	42.481
1200	20.790	44.423	29.931	17.390	-258.780	-209.714	38.194
1300	20.891	46.091	31.111	19.474	-258.467	-205.639	34.571
1400	21.019	47.644	32.237	21.570	-258.150	-201.586	31.469
1408	21.034	47.764	32.325	21.738	-258.124	-201.263	31.240
1408	21.034	47.764	32.325	21.738	-260.309	-201.263	31.240
1500	21.210	49.100	33.313	23.680	-260.238	-197.408	28.762
1600	21.496	50.477	34.343	25.815	-260.143	-193.221	26.392
1700	21.908	51.792	35.331	27.984	-260.019	-189.042	24.303
1800	22.476	53.060	36.281	30.202	-259.852	-184.871	22.446
1900	23.224	54.294	37.197	32.485	-259.626	-180.711	20.786
2000	24.168	55.508	38.082	34.853	-259.320	-176.566	19.294
2100	25.321	56.714	38.940	37.326	-258.915	-172.435	17.945
2200	26.685	57.923	39.776	39.924	-258.390	-168.331	16.722
2300	28.255	59.143	40.591	42.669	-257.724	-164.252	15.607
2400	30.012	60.382	41.390	45.581	-256.896	-160.205	14.588
2500	31.927	61.646	42.175	48.677	-255.889	-156.197	13.655
2600	33.958	62.937	42.949	51.970	-254.690	-152.232	12.796
2700	36.047	64.258	43.713	55.471	-253.288	-148.317	12.005
2800	38.120	65.606	44.471	59.179	-251.684	-144.455	11.275
2900	40.088	66.979	45.223	63.091	-249.881	-140.658	10.600
3000	41.840	68.368	45.971	67.190	-247.896	-136.926	9.975

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.
3115 K, melting point of UO_2; ΔH° = 18.176 kcal/mol.

UO_2(c) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 18.618 + 2.146\times10^{-3}T - 3.605\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.618\times10^{-3}T + 1.073\times10^{-6}T^2 + 3.605\times10^{2}T^{-1} - 6.855$

2000-3115 K: $Cp^\circ = -42.810 + 26.080\times10^{-3}T + 592.749\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = -42.810\times10^{-3}T + 13.040\times10^{-6}T^2 - 592.749\times10^{2}T^{-1} + 97.950$

3115-3600 K: $Cp^\circ = 31.440$

$H^\circ - H^\circ_{298} = 31.440\times10^{-3}T - 7.662$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf^\circ = -262.694 + 8.278\times10^{-3}T - 3.652\times10^{-6}T^2 + 402.800T^{-1}$

$\Delta Gf^\circ = -262.694 - 8.278\times10^{-3}T\ln T + 3.652\times10^{-6}T^2 + 201.400T^{-1} + 98.126\times10^{-3}T$

942-1049 K: $\Delta Hf^\circ = -260.284 + 1.133\times10^{-3}T + 0.570\times10^{-6}T^2 + 315.300T^{-1}$

$\Delta Gf^\circ = -260.284 - 1.133\times10^{-3}T\ln T - 0.570\times10^{-6}T^2 + 157.650T^{-1} + 50.665\times10^{-3}T$

1049-1408 K: $\Delta Hf^\circ = -262.581 + 2.238\times10^{-3}T + 0.570\times10^{-6}T^2 + 315.300T^{-1}$

$\Delta Gf^\circ = -262.581 - 2.238\times10^{-3}T\ln T - 0.570\times10^{-6}T^2 + 157.650T^{-1} + 60.539\times10^{-3}T$

1408-2000 K: $\Delta Hf^\circ = -261.274 - 0.242\times10^{-3}T + 0.570\times10^{-6}T^2 + 315.300T^{-1}$

$\Delta Gf^\circ = -261.274 + 0.242\times10^{-3}T\ln T - 0.570\times10^{-6}T^2 + 157.650T^{-1} + 41.631\times10^{-3}T$

2000-3000 K: $\Delta Hf^\circ = -155.132 - 62.780\times10^{-3}T + 12.831\times10^{-6}T^2 - 59904.900T^{-1}$

$\Delta Gf^\circ = -155.132 + 62.780\times10^{-3}T\ln T - 12.831\times10^{-6}T^2 - 29952.450T^{-1} - 454.735\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Huber (98). Low-temperature heat capacities and entropy at 298 K from Huntzicker (100). High-temperature data based on Moore (161), Gronvold (85), Ogard (169), Hein (93), and Liebowitz (142,143).

$UO_3(\gamma)$

Uranium Trioxide

[Formation: $U(c) + 1.5O_2(g) = UO_3(c)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	19.520	22.970	22.970	0	-292.570	-273.924	200.789
300	19.567	23.091	22.971	.036	-292.565	-273.808	199.467
400	21.311	28.997	23.764	2.093	-292.260	-267.601	146.208
500	22.213	33.857	25.311	4.273	-291.912	-261.475	114.289
600	22.801	37.962	27.087	6.525	-291.590	-255.419	93.035
700	23.241	41.512	28.901	8.828	-291.322	-249.412	77.869
800	23.602	44.639	30.675	11.171	-291.129	-243.441	66.504
900	23.917	47.438	32.386	13.547	-291.023	-237.486	57.669

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp° = 22.574 + 1.880\times10^{-3}T - 3.214\times10^{5}T^{-2}$

$H°-H°_{298} = 22.574\times10^{-3}T + 0.940\times10^{-6}T^{2} + 3.214\times10^{2}T^{-1} - 7.892$

Formation equations (kcal/mol):

298.15-900 K: $\Delta Hf° = -295.925 + 8.619\times10^{-3}T - 4.036\times10^{-6}T^{2} + 341.100T^{-1}$

$\Delta Gf° = -295.925 - 8.619\times10^{-3}T\ln T + 4.036\times10^{-6}T^{2} + 170.550T^{-1} + 119.776\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (105). Low-temperature heat capacities and entropy at 298 K from Westrum (244). High-temperature data based on Moore (161).

$U_4O_9(c)$

Tetrauranium Enneaoxide

[Formation: $4U(c,1) + 4.5O_2(g) = U_4O_9(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	70.400	79.880	79.880	0	-1078.100	-1021.856	749.031
300	70.760	80.280	79.880	.128	-1078.078	-1021.497	744.151
348	98.400	92.120	80.741	3.960	-1077.066	-1012.518	635.870
400	74.640	102.640	82.960	7.872	-1076.274	-1002.953	547.981
500	77.600	119.720	88.680	15.520	-1074.859	-984.797	430.449
600	79.560	134.040	95.080	23.376	-1073.589	-966.908	352.192
700	81.480	146.440	101.543	31.428	-1072.510	-949.206	296.352
800	83.400	157.480	107.890	39.672	-1071.668	-931.688	254.522
900	85.360	167.400	113.947	48.108	-1071.091	-914.211	221.998
942	86.183	171.312	116.418	51.710	-1070.938	-906.896	210.403
942	86.183	171.312	116.418	51.710	-1073.606	-906.896	210.403
1000	87.320	176.480	119.740	56.740	-1073.121	-896.634	195.957
1049	88.300	180.681	122.489	61.043	-1072.670	-887.993	185.003
1049	88.300	180.681	122.489	61.043	-1077.218	-887.993	185.003
1100	89.320	184.920	125.309	65.572	-1076.488	-878.837	174.607
1200	91.400	192.760	130.587	74.608	-1074.928	-860.911	156.791
1300	93.560	200.160	135.658	83.852	-1073.197	-843.150	141.745
1400	95.800	207.200	140.537	93.320	-1071.276	-825.548	128.872
1400	98.800	209.160	140.537	96.080	-1068.516	-825.548	128.872
1408	98.800	209.723	140.923	96.870	-1068.330	-824.151	127.923
1408	98.800	209.723	140.923	96.870	-1077.070	-824.151	127.923
1500	98.800	215.960	145.320	105.960	-1075.863	-807.642	117.672
1600	98.800	222.360	149.960	115.840	-1074.582	-789.844	107.886

Phase changes: 348 K, second order transition point of U_4O_9; $\Delta H° = 0$ kcal/mol.
942 K, α - β transition point of U; $\Delta H° = 0.667$ kcal/mol.
1049 K, β - γ transition point of U; $\Delta H° = 1.137$ kcal/mol.
1400 K, transition point of U_4O_9; $\Delta H° = 2.670$ kcal/mol.
1408 K, melting point of U; $\Delta H° = 2.185$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-348 K: $Cp° = -37.714 + 362.620\times10^{-3}T$

$H°- H°_{298} = -37.714\times10^{-3}T + 181.310\times10^{-6}T^2 - 4.873$

348-1400 K: $Cp° = 67.585 + 19.860\times10^{-3}T$

$H°- H°_{298} = 67.585\times10^{-3}T + 9.930\times10^{-6}T^2 - 20.762$

1400-1600 K: $Cp° = 98.800$

$H°- H°_{298} = 98.800\times10^{-3}T - 42.240$

U_4O_9(c) - Continued

Formation equations (kcal/mol):

298.15-348 K: $\Delta Hf^\circ = -1068.353 - 82.689\times10^{-3}T + 162.158\times10^{-6}T^2 + 146.600T^{-1}$

$\Delta Gf^\circ = -1068.353 + 82.689\times10^{-3}T\ln T - 162.158\times10^{-6}T^2 + 73.300T^{-1} - 267.655\times10^{-3}T$

348-942 K: $\Delta Hf^\circ = -1084.242 + 22.610\times10^{-3}T - 9.221\times10^{-6}T^2 + 146.600T^{-1}$

$\Delta Gf^\circ = -1084.242 - 22.610\times10^{-3}T\ln T + 9.221\times10^{-6}T^2 + 73.300T^{-1} + 334.594\times10^{-3}T$

942-1049 K: $\Delta Hf^\circ = -1074.602 - 5.970\times10^{-3}T + 7.667\times10^{-6}T^2 - 203.400T^{-1}$

$\Delta Gf^\circ = -1074.602 + 5.970\times10^{-3}T\ln T - 7.667\times10^{-6}T^2 - 101.700T^{-1} + 144.750\times10^{-3}T$

1049-1400 K: $\Delta Hf^\circ = -1083.786 - 1.550\times10^{-3}T + 7.667\times10^{-6}T^2 - 203.400T^{-1}$

$\Delta Gf^\circ = -1083.786 + 1.550\times10^{-3}T\ln T - 7.667\times10^{-6}T^2 - 101.700T^{-1} + 184.249\times10^{-3}T$

1400-1408 K: $\Delta Hf^\circ = -1105.265 + 29.665\times10^{-3}T - 2.263\times10^{-6}T^2 - 203.400T^{-1}$

$\Delta Gf^\circ = -1105.265 - 29.665\times10^{-3}T\ln T + 2.263\times10^{-6}T^2 - 101.700T^{-1} + 411.817\times10^{-3}T$

1408-1600 K: $\Delta Hf^\circ = -1100.037 + 19.745\times10^{-3}T - 2.263\times10^{-6}T^2 - 203.400T^{-1}$

$\Delta Gf^\circ = -1100.037 - 19.745\times10^{-3}T\ln T + 2.263\times10^{-6}T^2 - 101.700T^{-1} + 336.185\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Fitzgibbon (65). Low-temperature heat capacities and entropy at 298 K based on Osborne (173) and Flotow (68). High-temperature data based on Gronvold (85) and MacLeod (146).

V(c,l)

Vanadium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.950	6.915	6.915	0
300	5.958	6.952	6.915	.011
400	6.270	8.713	7.153	.624
500	6.440	10.131	7.611	1.260
600	6.570	11.317	8.134	1.910
700	6.700	12.339	8.662	2.574
800	6.850	13.243	9.179	3.251
900	7.020	14.060	9.678	3.944
1000	7.190	14.808	10.153	4.655
1100	7.380	15.502	10.608	5.383
1200	7.600	16.154	11.044	7.825
1300	7.825	16.771	11.461	6.903
1400	8.080	17.360	11.861	7.698
1500	8.320	17.926	12.247	8.518
1600	8.570	18.470	12.618	9.363
1700	8.850	18.998	12.978	10.234
1800	9.130	19.512	13.328	11.132
1900	9.450	20.014	13.666	12.061
2000	9.780	20.507	13.996	13.022
2100	10.150	20.993	14.318	14.018
2190	10.550	21.426	14.600	14.949
2190	11.043	23.920	14.600	20.410
2200	11.043	23.970	14.643	20.520
2300	11.043	24.461	15.059	21.624
2400	11.043	24.931	15.461	22.728
2500	11.043	25.382	15.849	23.832
2600	11.043	25.815	16.224	24.937
2700	11.043	26.232	16.587	26.041
2800	11.043	26.633	16.938	27.145
2900	11.043	27.021	17.280	28.250
3000	11.043	27.395	17.610	29.354

Phase changes: 2190 K, melting point of V; ΔH° = 5.461 kcal/mol.
3694 K, boiling point of V; ΔH° = 106.8 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2190 K: $Cp^\circ = 5.111 + 2.224\times10^{-3}T + 0.157\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.111\times10^{-3}T + 1.112\times10^{-6}T^2 - 0.157\times10^{2}T^{-1} - 1.570$

2190-3000 K: $Cp^\circ = 11.043$

$H^\circ - H^\circ_{298} = 11.043\times10^{-3}T - 3.774$

Source: Data from Chase (33).

V(g)

Vanadium (ideal monatomic gas)

[Formation: V(c,1) = V(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	6.217	43.544	43.544	0	123.200	112.279	-82.302
300	6.209	43.582	43.545	.011	123.200	112.211	-81.745
400	5.891	45.319	43.782	.615	123.191	108.549	-59.307
500	5.783	46.619	44.225	1.197	123.137	104.893	-45.848
600	5.804	47.674	44.716	1.775	123.065	101.251	-36.880
700	5.875	48.573	45.203	2.359	122.985	97.621	-30.478
800	5.949	49.363	45.675	2.950	122.899	94.003	-25.680
900	6.003	50.067	46.125	3.548	122.804	90.398	-21.951
1000	6.032	50.701	46.551	4.150	122.695	86.802	-18.970
1100	6.038	51.276	46.954	4.754	122.571	83.220	-16.534
1200	6.026	51.801	47.337	5.357	122.425	79.649	-14.506
1300	6.003	52.283	47.699	5.959	122.256	76.090	-12.792
1400	5.974	52.727	48.043	6.558	122.060	72.546	-11.325
1500	5.942	53.138	48.369	7.153	121.835	69.017	-10.056
1600	5.912	53.520	48.679	7.746	121.583	65.503	-8.947
1700	5.886	53.878	48.974	8.336	121.302	62.006	-7.971
1800	5.865	54.214	49.257	8.923	120.991	58.527	-7.106
1900	5.850	54.530	49.525	9.509	120.648	55.068	-6.334
2000	5.842	54.830	49.783	10.094	120.272	51.626	-5.641
2100	5.843	55.115	50.030	10.678	119.860	48.204	-5.017
2190	5.850	55.360	50.245	11.203	119.454	45.139	-4.505
2190	5.850	55.360	50.245	11.203	113.993	45.139	-4.505
2200	5.851	55.387	50.268	11.262	113.942	44.825	-4.453
2300	5.868	55.648	50.497	11.848	113.424	41.694	-3.962
2400	5.893	55.898	50.716	12.436	112.908	38.587	-3.514
2500	5.926	56.139	50.928	13.027	112.395	35.503	-3.104
2600	5.968	56.372	51.133	13.622	111.885	32.437	-2.727
2700	6.018	56.598	51.331	14.221	111.380	29.392	-2.379
2800	6.076	56.818	51.523	14.826	110.881	26.363	-2.058
2900	6.142	57.033	51.710	15.436	110.386	23.351	-1.760
3000	6.216	57.242	51.891	16.054	109.900	20.359	-1.483

Phase change: 2190 K, melting point of V; ΔH° = 5.461 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 5.681 + 0.130\times10^{-3}T + 0.442\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.681\times10^{-3}T + 0.065\times10^{-6}T^2 - 0.442\times10^{2}T^{-1} - 1.551$

Formation equations (kcal/mol):

298.15-2190 K: $\Delta Hf^\circ = 123.219 + 0.570\times10^{-3}T - 1.047\times10^{-6}T^2 - 28.500T^{-1}$

$\Delta Gf^\circ = 123.219 - 0.570\times10^{-3}T\ln T + 1.047\times10^{-6}T^2 - 14.250T^{-1} - 33.596\times10^{-3}T$

2190-3000 K: $\Delta Hf^\circ = 125.423 - 5.362\times10^{-3}T + 0.065\times10^{-6}T^2 - 44.200T^{-1}$

$\Delta Gf^\circ = 125.423 + 5.362\times10^{-3}T\ln T - 0.065\times10^{-6}T^2 - 22.100T^{-1} - 77.792\times10^{-3}T$

Source: Data from Chase (33).

VO(c)

Vanadium Oxide

[Formation: $V(c) + 0.5O_2(g) = VO(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.861	9.300	9.300	0	-103.200	-96.606	70.813
300	10.892	9.367	9.300	.020	-103.198	-96.565	70.346
400	11.873	12.660	9.743	1.167	-103.018	-94.379	51.566
500	12.373	15.366	10.604	2.381	-102.806	-92.243	40.319
600	12.800	17.660	11.595	3.639	-102.576	-90.152	32.837
700	13.218	19.664	12.607	4.940	-102.327	-88.101	27.506
800	13.631	21.456	13.602	6.283	-102.061	-86.087	23.518
900	14.037	23.085	14.567	7.666	-101.777	-84.106	20.424
1000	14.431	24.585	15.495	9.090	-101.478	-82.160	17.956
1100	14.809	25.978	16.385	10.552	-101.163	-80.243	15.943
1200	15.168	27.282	17.240	12.051	-100.837	-78.354	14.270
1300	15.508	28.510	18.060	13.585	-100.502	-76.495	12.860
1400	15.832	29.671	18.848	15.152	-100.162	-74.661	11.655
1500	16.145	30.774	19.607	16.751	-99.818	-72.851	10.614
1600	16.458	31.826	20.338	18.381	-99.472	-71.066	9.707
1700	16.788	32.834	21.044	20.043	-99.122	-69.302	8.909
1800	17.157	33.803	21.725	21.740	-98.767	-67.555	8.202

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 11.286 + 3.260\times10^{-3}T - 1.242\times10^{5}T^{-2}$

$H°- H°_{298} = 11.286\times10^{-3}T + 1.630\times10^{-6}T^{2} + 1.242\times10^{2}T^{-1} - 3.926$

Formation equations (kcal/mol):

298.15-1800 K: $\Delta Hf° = -104.380 + 2.560\times10^{-3}T + 0.267\times10^{-6}T^{2} + 117.300T^{-1}$

$\Delta Gf° = -104.380 - 2.560\times10^{-3}T\ln T - 0.267\times10^{-6}T^{2} + 58.650T^{-1} + 40.082\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (238). Low-temperature heat capacities and entropy at 298 K from Todd (223). High-temperature data based on Orr (172).

VO(g)

Vanadium Oxide (ideal gas)

[Formation: $V(c,l) + 0.5O_2(g) = VO(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.337	55.160	55.160	0	30.500	23.421	-17.168
300	7.344	55.205	55.160	.014	30.497	23.378	-17.031
400	7.710	57.369	55.451	.767	30.281	21.037	-11.494
500	8.011	59.123	56.017	1.553	30.066	18.750	-8.196
600	8.236	60.604	56.661	2.366	29.852	16.508	-6.013
700	8.400	61.887	57.318	3.198	29.631	14.301	-4.465
800	8.522	63.017	57.961	4.045	29.402	12.126	-3.313
900	8.614	64.026	58.579	4.902	29.159	9.983	-2.424
1000	8.685	64.938	59.171	5.767	28.899	7.864	-1.719
1100	8.741	65.768	59.733	6.638	28.623	5.774	-1.147
1200	8.786	66.531	60.268	7.515	28.326	3.711	-.676
1300	8.824	67.235	60.777	8.395	28.008	1.673	-.281
1400	8.856	67.891	61.263	9.279	27.664	-.342	.053
1500	8.884	68.502	61.725	10.166	27.297	-2.328	.339
1600	8.910	69.077	62.167	11.056	26.903	-4.293	.586
1700	8.934	69.618	62.590	11.948	26.483	-6.230	.801
1800	8.959	70.129	62.994	12.843	26.036	-8.139	.988
1900	8.984	70.614	63.382	13.740	25.557	-10.025	1.153
2000	9.010	71.075	63.755	14.640	25.046	-11.883	1.299
2100	9.039	71.516	64.115	15.542	24.500	-13.718	1.428
2190	9.067	71.896	64.427	16.356	23.974	-15.347	1.532
2190	9.067	71.896	64.427	16.356	18.513	-15.347	1.532
2200	9.070	71.937	64.461	16.447	18.448	-15.501	1.540
2300	9.104	72.341	64.795	17.356	17.795	-17.029	1.618
2400	9.142	72.729	65.117	18.268	17.142	-18.529	1.687
2500	9.183	73.103	65.429	19.185	16.493	-20.000	1.748
2600	9.228	73.464	65.731	20.105	15.842	-21.448	1.803
2700	9.277	73.813	66.024	21.030	15.195	-22.870	1.851
2800	9.329	74.152	66.309	21.961	14.552	-24.269	1.894
2900	9.385	74.480	66.585	22.896	13.909	-25.643	1.932
3000	9.444	74.799	66.853	23.838	13.271	-26.997	1.967

Phase change: 2190 K, melting point of V; $\Delta H° = 5.461$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 8.208 + 0.452\times10^{-3}T - 0.893\times10^{5}T^{-2}$

$H°- H°_{298} = 8.208\times10^{-3}T + 0.226\times10^{-6}T^{2} + 0.893\times10^{2}T^{-1} - 2.767$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 30.479 - 0.518\times10^{-3}T - 1.137\times10^{-6}T^{2} + 82.400T^{-1}$

$\Delta Gf° = 30.479 + 0.518\times10^{-3}T\ln T + 1.137\times10^{-6}T^{2} + 41.200T^{-1} - 27.427\times10^{-3}T$

2000-2190 K: $\Delta Hf° = 31.147 - 1.073\times10^{-3}T - 0.990\times10^{-6}T^{2} - 210.000T^{-1}$

$\Delta Gf° = 31.147 + 1.073\times10^{-3}T\ln T + 0.990\times10^{-6}T^{2} - 105.000T^{-1} - 31.649\times10^{-3}T$

2190-3000 K: $\Delta Hf° = 33.351 - 7.005\times10^{-3}T + 0.121\times10^{-6}T^{2} - 225.700T^{-1}$

$\Delta Gf° = 33.351 + 7.005\times10^{-3}T\ln T - 0.121\times10^{-6}T^{2} - 112.850T^{-2} - 75.845\times10^{-3}T$

Source: Data from Chase (33).

$V_2O_3(c)$

Divanadium Trioxide

[Formation: $2V(c) + 1.5O_2(g) = V_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	25.250	23.500	23.500	0	-293.500	-274.467	201.187
300	25.234	23.656	23.500	.047	-293.495	-274.348	199.860
400	28.075	31.358	24.533	2.730	-293.102	-268.021	146.438
500	29.612	37.802	26.560	5.621	-292.580	-261.809	114.435
600	30.599	43.294	28.902	8.635	-291.999	-255.707	93.140
700	31.302	48.066	31.306	11.732	-291.397	-249.707	77.961
800	31.855	52.283	33.671	14.890	-290.789	-243.795	66.601
900	32.344	56.064	35.952	18.101	-290.185	-237.954	57.782
1000	32.839	59.497	38.138	21.359	-289.590	-232.186	50.744
1100	33.399	62.652	40.224	24.671	-288.993	-226.472	44.995
1200	34.074	65.586	42.217	28.043	-288.391	-220.814	40.215
1300	34.899	68.345	44.122	31.490	-287.770	-215.208	36.179
1400	35.894	70.967	45.947	35.028	-287.118	-209.652	32.728
1500	37.055	73.482	47.699	38.675	-286.415	-204.141	29.743
1600	38.351	75.914	49.387	42.444	-285.652	-198.685	27.139
1700	39.717	78.280	51.017	46.347	-284.814	-193.274	24.847
1800	41.047	80.588	52.596	50.386	-283.903	-187.911	22.815

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 28.574 + 5.202\times10^{-3}T - 4.334\times10^{5}T^{-2}$

$H°- H°_{298} = 28.574\times10^{-3}T + 2.601\times10^{-6}T^{2} + 4.334\times10^{2}T^{-1} - 10.204$

Formation equations (kcal/mol):

298.15-1800 K: $\Delta Hf° = -297.036 + 7.507\times10^{-3}T - 0.377\times10^{-6}T^{2} + 397.000T^{-1}$

$\Delta Gf° = -297.036 - 7.507\times10^{-3}T\ln T + 0.377\times10^{-6}T^{2} + 198.500T^{-1} + 116.124\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (238). Low-temperature-heat capacities and entropy at 298 K from Anderson (5). High-temperature data based on Cook (41).

$V_2O_4(c,1)$

Divanadium Tetroxide

[Formation: $2V(c) + 2O_2(g) = V_2O_4(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	27.958	24.600	24.600	0	-341.100	-315.089	230.964
300	28.060	24.773	24.600	.052	-341.096	-314.927	229.421
340	30.240	28.419	24.836	1.218	-340.976	-311.445	200.192
340	31.695	34.601	24.836	3.320	-338.874	-311.445	200.192
400	32.653	39.835	26.702	5.253	-338.541	-306.633	167.534
500	33.849	47.251	30.093	8.579	-337.949	-298.723	130.570
600	35.054	53.529	33.489	12.024	-337.314	-290.935	105.972
700	36.234	59.022	36.752	15.589	-336.633	-283.259	88.436
800	37.280	63.931	39.848	19.266	-335.906	-275.686	75.313
900	38.121	68.372	42.774	23.038	-335.148	-268.201	65.127
1000	38.735	72.423	45.541	26.882	-334.380	-260.807	56.999
1100	39.137	76.135	48.155	30.778	-333.618	-253.484	50.362
1200	39.375	79.551	50.631	34.704	-332.886	-246.230	44.844
1300	39.521	82.709	52.978	38.650	-332.194	-239.037	40.185
1400	39.664	85.643	55.209	42.608	-331.554	-231.898	36.200
1500	39.909	88.387	57.330	46.586	-330.956	-224.800	32.753
1600	40.366	90.976	59.353	50.597	-330.389	-217.746	29.742
1700	41.154	93.445	61.286	54.670	-329.822	-210.722	27.090
1800	42.388	95.830	63.139	58.843	-329.221	-203.729	24.736
1818	42.667	96.252	63.464	59.608	-329.107	-202.473	24.340
1818	51.000	111.215	63.464	86.810	-301.905	-202.473	24.340
1900	51.000	113.465	65.574	90.992	-300.718	-198.017	22.777
2000	51.000	116.081	68.035	96.092	-299.338	-192.648	21.051

Phase changes: 340 K, α - β transition point of V_2O_4; $\Delta H° = 2.102$ kcal/mol.
1818 K, melting point of V_2O_4; $\Delta H° = 27.202$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-340 K:
$$Cp° = 11.704 + 54.528\times10^{-3}T$$
$$H°- H°_{298} = 11.704\times10^{-3}T + 27.264\times10^{-6}T^2 - 5.913$$

340-1818 K:
$$Cp° = 33.544 + 4.812\times10^{-3}T - 4.029\times10^{5}T^{-2}$$
$$H°- H°_{298} = 33.544\times10^{-3}T + 2.406\times10^{-6}T^2 + 4.029\times10^{2}T^{-1} - 9.548$$

1818-2000 K:
$$Cp° = 51.000$$
$$H°- H°_{298} = 51.000\times10^{-3}T - 5.908$$

Formation equations (kcal/mol):

298.15-340 K:
$$\Delta Hf° = -339.169 - 12.978\times10^{-3}T + 24.034\times10^{-6}T^2 - 59.000T^{-1}$$
$$\Delta Gf° = -339.169 + 12.978\times10^{-3}T\ln T - 24.034\times10^{-6}T^2 - 29.500T^{-1} + 14.318\times10^{-3}T$$

340-1818 K:
$$\Delta Hf° = -342.804 + 8.862\times10^{-3}T - 0.824\times10^{-6}T^2 + 343.900T^{-1}$$
$$\Delta Gf° = -342.804 - 8.862\times10^{-3}T\ln T + 0.824\times10^{-6}T^2 + 171.950T^{-1} + 142.119\times10^{-3}T$$

1818-2000 K:
$$\Delta Hf° = -339.164 + 26.318\times10^{-3}T - 3.230\times10^{-6}T^2 - 59.000T^{-1}$$
$$\Delta Gf° = -339.164 - 26.318\times10^{-3}T\ln T + 3.230\times10^{-6}T^2 - 29.500T^{-1} + 266.820\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Wagman (238). Low-temperature heat capacities and entropy at 298 K from Anderson (5). High-temperature data based on Cook (41).

$V_2O_5(c,l)$

Divanadium Pentoxide

[Formation: $2V(c) + 2.5O_2g) = V_2O_5(c,l)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	30.500	31.140	31.140	0	-370.600	-339.234	248.662
300	30.609	31.329	31.140	.057	-370.598	-339.038	246.986
400	34.519	40.752	32.399	3.341	-370.315	-328.555	179.512
500	36.516	48.687	34.885	6.901	-369.854	-318.165	139.068
600	37.978	55.478	37.765	10.628	-369.315	-307.875	112.142
700	39.364	61.435	40.729	14.494	-368.722	-297.683	92.940
800	40.866	66.788	43.658	18.504	-368.061	-287.582	78.563
900	42.577	71.698	46.504	22.675	-367.311	-277.563	67.401
950	43.527	74.025	47.891	24.827	-366.895	-272.591	62.709
950	45.500	90.176	47.891	40.170	-351.552	-272.591	62.709
1000	45.500	92.509	50.064	42.445	-351.030	-268.448	58.669
1100	45.500	96.846	54.123	46.995	-350.034	-260.237	51.704
1200	45.500	100.805	57.851	51.545	-349.102	-252.114	45.916
1300	45.500	104.447	61.297	56.095	-348.234	-244.068	41.031
1400	45.500	107.819	64.501	60.645	-347.434	-236.087	36.854
1500*	45.500	110.958	67.495	65.195	-346.698	-228.159	33.242

*V_2O_5 decomposes above 1500 K.

Phase change: 950 K melting point of V_2O_5; ΔH° = 15.343 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-950 K: $Cp^\circ = 34.065 + 9.690\times10^{-3}T - 5.737\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 34.065\times10^{-3}T + 4.845\times10^{-6}T^2 + 5.737\times10^{2}T^{-1} - 12.511$

950-1500 K: $Cp^\circ = 45.500$

$H^\circ - H^\circ_{298} = 45.500\times10^{-3}T - 3.055$

Formation equations (kcal/mol):

298.15-950 K: $\Delta Hf^\circ = -374.091 + 5.768\times10^{-3}T + 1.363\times10^{-6}T^2 + 492.100T^{-1}$

$\Delta Gf^\circ = -374.091 - 5.768\times10^{-3}T\ln T - 1.363\times10^{-6}T^2 + 246.050T^{-1} + 147.415\times10^{-3}T$

950-1500 K: $\Delta Hf^\circ = -364.635 + 17.203\times10^{-3}T - 3.481\times10^{-6}T^2 - 81.600T^{-1}$

$\Delta Gf^\circ = -364.635 - 17.203\times10^{-3}T\ln T + 3.481\times10^{-6}T^2 - 40.800T^{-1} + 211.580\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (238). Low-temperature heat capacities and entropy at 298 K from Sukhovei (215). High-temperature data based on Slyusar (205).

W(c)

Tungsten

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	5.800	7.800	7.800	0
300	5.800	7.840	7.803	.011
400	6.000	9.540	8.035	.602
500	6.120	10.890	8.474	1.208
600	6.220	12.010	8.967	1.826
700	6.300	12.980	9.477	2.452
800	6.370	13.820	9.965	3.084
900	6.430	14.580	10.441	3.725
1000	6.500	15.260	10.890	4.370
1100	6.580	15.890	11.324	5.023
1200	6.660	16.460	11.722	5.685
1300	6.740	17.000	12.112	6.354
1400	6.830	17.510	12.486	7.033
1500	6.910	17.980	12.834	7.719
1600	6.990	18.430	13.171	8.414
1700	7.060	18.860	13.498	9.116
1800	7.140	19.260	13.801	9.827
1900	7.220	19.650	14.100	10.545
2000	7.300	20.020	14.384	11.272
2100	7.380	20.380	14.662	12.007
2200	7.460	20.720	14.925	12.749
2300	7.540	21.050	15.181	13.499
2400	7.630	21.380	15.440	14.257
2500	7.710	21.700	15.690	15.024
2600	7.780	22.000	15.923	15.799
2700	7.860	22.290	16.149	16.581
2800	7.940	22.580	16.376	17.370
2900	8.020	22.860	16.595	18.168
3000	8.100	23.140	16.815	18.976

Phase change: 3680 K, melting point of W; ΔH° = 8.5 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 5.815 + 0.742\times10^{-3}T - 0.210\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.815\times10^{-3}T + 0.371\times10^{-6}T^2 + 0.210\times10^{5}T^{-1} - 1.837$

Source: Data from Hultgren (99) corrected to IPTS-68.

W(g)

Tungsten (ideal monatomic gas)

[Formation: W(c) = W(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	5.092	41.549	41.549	0	203.400	193.338	-141.719
300	5.097	41.581	41.551	.009	203.398	193.276	-140.799
400	5.536	43.099	41.754	.538	203.336	189.912	-103.762
500	6.296	44.411	42.157	1.127	203.319	186.559	-81.544
600	7.251	45.641	42.634	1.804	203.378	183.199	-66.729
700	8.217	46.833	43.150	2.578	203.526	179.829	-56.144
800	9.026	47.985	43.683	3.442	203.758	176.426	-48.197
900	9.577	49.083	44.223	4.374	204.049	172.996	-42.009
1000	9.855	50.109	44.761	5.348	204.378	169.529	-37.050
1100	9.904	51.052	45.290	6.338	204.715	166.037	-32.988
1200	9.787	51.910	45.807	7.324	205.039	162.499	-29.595
1300	9.569	52.685	46.307	8.292	205.338	158.947	-26.721
1400	9.297	53.384	46.787	9.236	205.603	155.379	-24.256
1500	9.007	54.016	47.249	10.151	205.832	151.778	-22.114
1600	8.721	54.588	47.690	11.037	206.023	148.170	-20.239
1700	8.451	55.108	48.110	11.896	206.180	144.558	-18.584
1800	8.205	55.584	48.513	12.728	206.301	140.918	-17.110
1900	7.987	56.022	48.897	13.537	206.392	137.285	-15.791
2000	7.796	56.427	49.264	14.326	206.454	133.640	-14.603
2100	7.634	56.803	49.613	15.098	206.491	130.003	-13.529
2200	7.499	57.155	49.949	15.854	206.505	126.348	-12.551
2300	7.389	57.486	50.269	16.598	206.499	122.696	-11.659
2400	7.304	57.798	50.576	17.333	206.476	119.073	-10.843
2500	7.240	58.095	50.871	18.060	206.436	115.448	-10.092
2600	7.197	58.378	51.155	18.781	206.382	111.799	-9.397
2700	7.174	58.649	51.427	19.500	206.319	108.150	-8.754
2800	7.167	58.910	51.690	20.217	206.247	104.523	-8.158
2900	7.176	59.162	51.943	20.934	206.166	100.890	-7.603
3000	7.200	59.405	52.188	21.652	206.076	97.281	-7.087

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 7.894 + 0.604\times10^{-3}T - 2.651\times10^{5}T^{-2}$

$H°- H°_{298} = 7.894\times10^{-3}T + 0.302\times10^{-6}T^{2} + 2.651\times10^{2}T^{-1} - 3.270$

Formation equations (kcal/mol):

298.15-3000 K: $\Delta Hf° = 201.968 + 2.079\times10^{-3}T - 0.069\times10^{-6}T^{2} + 244.100T^{-1}$

$\Delta Gf° = 201.968 - 2.079\times10^{-3}T\ln T + 0.069\times10^{-6}T^{2} + 122.050T^{-1} - 18.493\times10^{-3}T$

Source: Data from JANAF (51).

WO(g)

Tungsten Oxide (ideal gas)

[Formation: $W(c) + 0.5O_2(g) = WO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.287	58.722	58.722	0	108.000	100.123	-73.391
300	7.294	58.767	58.724	.013	107.995	100.075	-72.903
400	7.646	60.914	59.012	.761	107.798	97.466	-53.252
500	7.947	62.654	59.572	1.541	107.606	94.904	-41.482
600	8.176	64.124	60.211	2.348	107.418	92.378	-33.648
700	8.346	65.398	60.864	3.174	107.229	89.890	-28.064
800	8.472	66.521	61.502	4.015	107.038	87.422	-23.882
900	8.567	67.524	62.116	4.867	106.842	84.986	-20.637
1000	8.640	68.431	62.703	5.728	106.645	82.569	-18.045
1100	8.698	69.257	63.262	6.595	106.439	80.180	-15.930
1200	8.744	70.016	63.793	7.467	106.226	77.795	-14.168
1300	8.781	70.717	64.299	8.343	106.005	75.441	-12.683
1400	8.813	71.369	64.781	9.223	105.773	73.108	-11.413
1500	8.839	71.978	65.241	10.106	105.535	70.778	-10.312
1600	8.862	72.549	65.680	10.991	105.287	68.472	-9.353
1700	8.881	73.087	66.100	11.878	105.031	66.186	-8.509
1800	8.899	73.595	66.502	12.767	104.765	63.898	-7.758
1900	8.915	74.077	66.889	13.658	104.491	61.637	-7.090
2000	8.930	74.535	67.260	14.550	104.207	59.382	-6.489

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.957 + 0.670\times10^{-3}T - 0.773\times10^{5}T^{-2}$

$H°- H°_{298} = 7.957\times10^{-3}T + 0.335\times10^{-6}T^{2} + 0.773\times10^{2}T^{-1} - 2.661$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 108.352 - 1.473\times10^{-3}T - 0.288\times10^{-6}T^{2} + 33.700T^{-1}$

$\Delta Gf° = 108.352 + 1.473\times10^{-3}T\ln T + 0.288\times10^{-6}T^{2} + 16.850T^{-1} - 36.267\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). All other data from JANAF (51).

$WO_2(c)$

Tungsten Dioxide

[Formation: $W(c) + O_2(g) = WO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.320	12.080	12.080	0	-140.940	-127.605	93.536
300	13.359	12.163	12.080	.025	-140.939	-127.521	92.898
400	15.121	16.271	12.628	1.457	-140.808	-123.064	67.238
500	16.279	19.778	13.718	3.030	-140.572	-118.656	51.864
600	17.077	22.820	14.985	4.701	-140.274	-114.302	41.634
700	17.643	25.498	16.301	6.438	-139.941	-109.996	34.342
800	18.055	27.882	17.602	8.224	-139.585	-105.747	28.888
900	18.365	30.027	18.865	10.046	-139.218	-101.533	24.655
1000	18.610	31.975	20.080	11.895	-138.841	-97.366	21.279
1100	18.828	33.759	21.244	13.767	-138.461	-93.228	18.522
1200	19.063	35.407	22.356	15.661	-138.077	-89.140	16.234
1300	19.367	36.944	23.419	17.582	-137.681	-85.071	14.302
1400	19.794	38.394	24.438	19.539	-137.267	-81.030	12.649
1500	20.394	39.779	25.415	21.546	-136.816	-77.035	11.224
1600	21.195	41.120	26.355	23.624	-136.310	-73.064	9.980
1700	22.183	42.434	27.262	25.792	-135.726	-69.120	8.886
1800	23.279	43.733	28.141	28.065	-135.052	-65.232	7.920

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 15.975 + 3.052\times10^{-3}T - 3.169\times10^{5}T^{-2}$

$H°- H°_{298} = 15.975\times10^{-3}T + 1.526\times10^{-6}T^{2} + 3.169\times10^{2}T^{-1} - 5.961$

Formation equations (kcal/mol):

298.15-1800 K: $\Delta Hf° = -142.712 + 2.930\times10^{-3}T + 0.652\times10^{-6}T^{2} + 250.700T^{-1}$

$\Delta Gf° = -142.712 - 2.930\times10^{-3}T\ln T - 0.652\times10^{-6}T^{2} + 125.350T^{-1} + 66.148\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). All other data based on King (134).

$WO_2(g)$

Tungsten Dioxide (ideal gas)

[Formation: $W(c) + O_2(g) = WO_2(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	10.471	68.209	68.209	0	11.000	7.600	-5.571
300	10.489	68.274	68.211	.019	10.995	7.579	-5.522
400	11.355	71.415	68.632	1.113	10.788	6.474	-3.537
500	11.999	74.022	69.456	2.283	10.621	5.415	-2.367
600	12.454	76.252	70.407	3.507	10.472	4.385	-1.597
700	12.776	78.197	71.384	4.769	10.330	3.385	-1.057
800	13.006	79.919	72.345	6.059	10.190	2.399	-.655
900	13.176	81.461	73.274	7.368	10.044	1.438	-.349
1000	13.303	82.856	74.163	8.693	9.897	.491	-.107
1100	13.401	84.129	75.013	10.028	9.740	-.434	.086
1200	13.477	85.299	75.822	11.372	9.574	-1.359	.248
1300	13.538	86.380	76.593	12.723	9.400	-2.257	.379
1400	13.587	87.385	77.329	14.079	9.213	-3.138	.490
1500	13.627	88.324	78.031	15.440	9.018	-4.018	.585
1600	13.660	89.204	78.701	16.805	8.811	-4.877	.666
1700	13.688	90.033	79.344	18.172	8.594	-5.718	.735
1800	13.711	90.816	79.959	19.542	8.365	-6.564	.797
1900	13.731	91.558	80.551	20.914	8.125	-7.385	.849
2000	13.748	92.263	81.119	22.288	7.873	-8.201	.896

*All data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.460 + 0.882\times10^{-3}T - 2.002\times10^{5}T^{-2}$

$H°- H°_{298} = 12.460\times10^{-3}T + 0.441\times10^{-6}T^{2} + 2.002\times10^{2}T^{-1} - 4.426$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 10.763 - 0.585\times10^{-3}T - 0.433\times10^{-6}T^{2} + 134.000T^{-1}$

$\Delta Gf° = 10.763 + 0.585\times10^{-3}T\ln T + 0.433\times10^{-6}T^{2} + 67.000T^{-1} - 14.827\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (237). All other data are those estimated by JANAF (51).

$WO_3(c,1)$

Tungsten Trioxide

[Formation: $W(c) + 1.5O_2(g) = WO_3(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.600	18.150	18.150	0	-201.480	-182.650	133.884
300	17.635	18.259	18.150	.033	-201.477	-182.531	132.972
400	19.696	23.645	18.873	1.909	-201.257	-176.245	96.295
500	21.218	28.212	20.294	3.959	-200.910	-170.030	74.319
600	22.247	32.179	21.952	6.136	-200.483	-163.898	59.699
700	22.872	35.659	23.666	8.395	-200.017	-157.832	49.277
800	23.249	38.740	25.363	10.702	-199.540	-151.844	41.481
900	23.558	41.496	27.005	13.042	-199.062	-145.905	35.430
1000	23.989	43.998	28.580	15.418	-198.571	-140.024	30.602
1051	24.316	45.190	29.357	16.640	-198.321	-137.036	28.496
1051	23.641	45.580	29.357	17.050	-197.911	-137.036	28.496
1100	23.769	46.670	30.105	18.221	-197.680	-134.204	26.664
1200	24.036	48.749	31.573	20.611	-197.224	-128.460	23.395
1300	24.310	50.684	32.970	23.028	-196.759	-122.743	20.635
1400	24.589	52.496	34.301	25.473	-196.290	-117.059	18.273
1500	24.873	54.202	35.571	27.946	-195.807	-111.421	16.234
1600	25.159	55.816	36.786	30.448	-195.316	-105.808	14.453
1700	25.448	57.350	37.951	32.978	-194.811	-100.221	12.884
1747	25.584	58.047	38.482	34.180	-194.567	-97.609	12.211
1747	31.400	68.093	38.482	51.730	-177.017	-97.609	12.211
1800	31.400	69.029	39.367	53.391	-176.441	-95.218	11.561
1900	31.400	70.727	40.974	56.531	-175.360	-90.733	10.437
2000	31.400	72.338	42.502	59.671	-174.295	-86.313	9.432

Phase changes: 1051 K, α - β transition point of WO_3; $\Delta H° = 0.410$ kcal/mol.
1747 K, melting point of WO_3; $\Delta H° = 17.550$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1051 K:
$$Cp° = 20.733 + 3.828\times10^{-3}T - 3.799\times10^{5}T^{-2}$$
$$H°- H°_{298} = 20.733\times10^{-3}T + 1.914\times10^{-6}T^{2} + 3.799\times10^{2}T^{-1} - 7.626$$

1051-1747 K:
$$Cp° = 21.591 + 2.332\times10^{-3}T - 4.423\times10^{5}T^{-2}$$
$$H°- H°_{298} = 21.591\times10^{-3}T + 1.166\times10^{-6}T^{2} + 4.423\times10^{2}T^{-1} - 7.351$$

1747-2000 K:
$$Cp° = 31.400$$
$$H°- H°_{298} = 31.400\times10^{-3}T - 3.126$$

Formation equations (kcal/mol):

298.15-1051 K:
$$\Delta Hf° = -203.741 + 4.073\times10^{-3}T + 0.788\times10^{-6}T^{2} + 291.100T^{-1}$$
$$\Delta Gf° = -203.741 - 4.073\times10^{-3}T\ln T - 0.788\times10^{-6}T^{2} + 145.550T^{-1} + 92.544\times10^{-3}T$$

1051-1747 K:
$$\Delta Hf° = -203.466 + 4.931\times10^{-3}T + 0.041\times10^{-6}T^{2} + 353.500T^{-1}$$
$$\Delta Gf° = -203.466 - 4.931\times10^{-3}T\ln T - 0.041\times10^{-6}T^{2} + 176.750T^{-1} + 97.438\times10^{-3}T$$

1747-2000 K:
$$\Delta Hf° = -199.240 + 14.740\times10^{-3}T - 1.126\times10^{-6}T^{2} - 88.800T^{-1}$$
$$\Delta Gf° = -199.240 - 14.740\times10^{-3}T\ln T + 1.126\times10^{-6}T^{2} - 44.400T^{-1} + 166.285\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Mah (148). All other data based on King (134).

$WO_3(g)$

Tungsten Trioxide (ideal gas)

[Formation: $W(c) + 1.5O_2(g) = WO_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	14.580	68.434	68.434	0	-70.000	-66.162	48.497
300	14.613	68.524	68.434	.027	-70.004	-66.137	48.180
400	16.071	72.941	69.026	1.566	-70.120	-64.827	35.419
500	17.065	76.641	70.189	3.226	-70.163	-63.498	27.754
600	17.746	79.816	71.536	4.968	-70.172	-62.168	22.644
700	18.219	82.589	72.920	6.768	-70.164	-60.830	18.992
800	18.557	85.045	74.285	8.608	-70.154	-59.502	16.255
900	18.805	87.246	75.605	10.477	-70.146	-58.165	14.124
1000	18.990	89.237	76.870	12.367	-70.142	-56.834	12.421
1100	19.133	91.054	78.079	14.273	-70.147	-55.494	11.026
1200	19.244	92.724	79.231	16.192	-70.163	-54.169	9.865
1300	19.332	94.268	80.329	18.121	-70.187	-52.830	8.881
1400	19.403	95.703	81.376	20.058	-70.225	-51.483	8.037
1500	19.461	97.044	82.377	22.001	-70.272	-50.149	7.307
1600	19.509	98.301	83.332	23.950	-70.334	-48.802	6.666
1700	19.549	99.485	84.248	25.903	-70.406	-47.446	6.099
1800	19.583	100.604	85.127	27.859	-70.493	-46.105	5.598
1900	19.612	101.663	85.969	29.819	-70.592	-44.743	5.147
2000	19.637	102.670	86.779	31.782	-70.705	-43.386	4.741
2100	19.658	103.629	87.559	33.746	-70.833	-42.015	4.372
2200	19.677	104.543	88.310	35.713	-70.973	-40.649	4.038
2300	19.693	105.419	89.036	37.682	-71.128	-39.278	3.732
2400	19.707	106.257	89.735	39.652	-71.298	-37.870	3.449
2500	19.720	107.062	90.413	41.623	-71.483	-36.457	3.187
2600	19.731	107.835	91.067	43.596	-71.681	-35.061	2.947
2700	19.741	108.580	91.703	45.569	-71.894	-33.665	2.725
2800	19.750	109.298	92.318	47.544	-72.120	-32.232	2.516
2900	19.758	109.992	92.916	49.519	-72.362	-30.806	2.322
3000	19.766	110.662	93.497	51.495	-72.620	-29.353	2.138

*All data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 18.146 + 0.886\times10^{-3}T - 3.405\times10^{5}T^{-2}$

$H°- H°_{298} = 18.146\times10^{-3}T + 0.443\times10^{-6}T^{2} + 3.405\times10^{2}T^{-1} - 6.592$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -71.227 + 1.486\times10^{-3}T - 0.683\times10^{-6}T^{2} + 251.700T^{-1}$

$\Delta Gf° = -71.227 - 1.486\times10^{-3}T\ln T + 0.683\times10^{-6}T^{2} + 125.850T^{-1} + 23.835\times10^{-3}T$

2000-3000 K: $\Delta Hf° = -69.222 - 0.179\times10^{-3}T - 0.242\times10^{-6}T^{2} - 625.500T^{-1}$

$\Delta Gf° = -69.222 + 0.179\times10^{-3}T\ln T + 0.242\times10^{-6}T^{2} - 312.750T^{-1} + 11.169\times10^{-3}T$

Source: Data from JANAF (51) who estimated all except enthalpy of formation at 298 K.

$(WO_3)_2(g)$

Dimeric Tungsten Trioxide (ideal gas)

[Formation: $2W(c) + 3O_2(g) = (WO_3)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	36.726	99.298	99.298	0	-278.200	-259.322	190.086
300	36.793	99.526	99.299	.068	-278.193	-259.203	188.827
400	39.407	110.510	100.780	3.892	-277.681	-252.945	138.201
500	40.814	119.469	103.649	7.910	-277.068	-246.831	107.888
600	41.642	126.990	106.930	12.036	-276.443	-240.850	87.729
700	42.165	133.451	110.268	16.228	-275.837	-234.959	73.357
800	42.515	139.106	113.527	20.463	-275.260	-229.169	62.605
900	42.759	144.128	116.652	24.728	-274.719	-223.429	54.255
1000	42.937	148.643	119.630	29.013	-274.205	-217.758	47.590
1100	43.069	152.742	122.457	33.314	-273.727	-212.118	42.143
1200	43.171	156.494	125.139	37.626	-273.283	-206.551	37.618
1300	43.251	159.953	127.686	41.947	-272.868	-200.996	33.790
1400	43.314	163.160	130.106	46.276	-272.489	-195.462	30.513
1500	43.366	166.151	132.411	50.610	-272.137	-189.985	27.680
1600	43.408	168.951	134.609	54.948	-271.820	-184.514	25.203
1700	43.443	171.583	136.706	59.291	-271.527	-179.049	23.018
1800	43.472	174.067	138.713	63.637	-271.267	-173.637	21.082
1900	43.497	176.418	140.636	67.985	-271.037	-168.215	19.349
2000	43.519	178.650	142.482	72.336	-270.837	-162.821	17.792
2100	43.537	180.774	144.255	76.689	-270.669	-157.416	16.382
2200	43.553	182.800	145.962	81.043	-270.529	-152.052	15.105
2300	43.567	184.736	147.606	85.399	-270.421	-146.686	13.938
2400	43.579	186.590	149.191	89.757	-270.342	-141.270	12.864
2500	43.590	188.370	150.724	94.115	-270.296	-135.861	11.877
2600	43.600	190.079	152.204	98.475	-270.279	-130.503	10.970
2700	43.608	191.725	153.638	102.835	-270.291	-125.158	10.131
2800	43.616	193.311	155.027	107.196	-270.331	-119.758	9.347
2900	43.623	194.842	156.374	111.558	-270.403	-114.380	8.620
3000	43.629	196.321	157.681	115.921	-270.509	-108.965	7.938

*All data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 43.030 + 0.336\times10^{-3}T - 5.692\times10^{5}T^{-2}$

$H°- H°_{298} = 43.030\times10^{-3}T + 0.168\times10^{-6}T^{2} + 5.692\times10^{2}T^{-1} - 14.753$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -282.223 + 9.710\times10^{-3}T - 2.083\times10^{-6}T^{2} + 391.600T^{-1}$

$\Delta Gf° = -282.223 - 9.710\times10^{-3}T\ln T + 2.083\times10^{-6}T^{2} + 195.800T^{-1} + 129.311\times10^{-3}T$

2000-3000 K: $\Delta Hf° = -278.214 + 6.380\times10^{-3}T - 1.201\times10^{-6}T^{2} - 1362.800T^{-1}$

$\Delta Gf° = -278.214 - 6.380\times10^{-3}T\ln T + 1.201\times10^{-6}T^{2} - 681.400T^{-1} + 103.979\times10^{-3}T$

Source: Data from JANAF (51) who estimated all except enthalpy of formation at 298 K.

$(WO_3)_3(g)$

Trimeric Tungsten Trioxide (ideal gas)

[Formation: $3W(c) + 4.5O_2(g) = (WO_3)_3(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	53.284	120.599	120.599	0	-483.600	-446.831	327.532
300	53.401	120.929	120.599	.099	-483.592	-446.599	325.343
400	58.219	137.015	122.760	5.702	-482.958	-434.354	237.317
500	61.048	150.337	126.983	11.677	-482.090	-422.301	184.585
600	62.806	161.634	131.841	17.876	-481.142	-410.443	149.502
700	63.956	171.408	136.811	24.218	-480.180	-398.725	124.486
800	64.742	180.003	141.683	30.656	-479.229	-387.167	105.768
900	65.301	187.662	146.374	37.159	-478.312	-375.699	91.231
1000	65.711	194.565	150.854	43.711	-477.416	-364.346	79.627
1100	66.020	200.843	155.118	50.298	-476.564	-353.053	70.144
1200	66.259	206.598	159.171	56.913	-475.751	-341.881	62.264
1300	66.446	211.909	163.026	63.548	-474.975	-330.740	55.602
1400	66.597	216.839	166.695	70.201	-474.247	-319.645	49.898
1500	66.719	221.438	170.193	76.867	-473.553	-308.643	44.969
1600	66.819	225.747	173.532	83.544	-472.908	-297.662	40.658
1700	66.903	229.801	176.725	90.230	-472.297	-286.705	36.858
1800	66.973	233.627	179.780	96.924	-471.732	-275.834	33.490
1900	67.033	237.250	182.711	103.624	-471.209	-264.959	30.477
2000	67.084	240.689	185.524	110.330	-470.730	-254.134	27.770
2100	67.128	243.963	188.229	117.041	-470.296	-243.301	25.320
2200	67.166	247.087	190.835	123.755	-469.903	-232.540	23.100
2300	67.200	250.074	193.346	130.474	-469.556	-221.784	21.074
2400	67.229	252.934	195.769	137.195	-469.254	-210.963	19.211
2500	67.255	255.679	198.111	143.919	-468.998	-200.155	17.497
2600	67.278	258.317	200.376	150.646	-468.785	-189.437	15.923
2700	67.299	260.857	202.570	157.375	-468.614	-178.742	14.468
2800	67.317	263.305	204.696	164.106	-468.485	-167.973	13.111
2900	67.334	265.667	206.757	170.838	-468.404	-157.241	11.850
3000	67.349	267.950	208.759	177.573	-468.372	-146.462	10.670

*All data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 64.890 + 1.390\times10^{-3}T - 10.686\times10^{5}T^{-2}$

$H°- H°_{298} = 64.890\times10^{-3}T + 0.695\times10^{-6}T^{2} + 10.686\times10^{2}T^{-1} - 22.993$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -490.498 + 14.910\times10^{-3}T - 2.681\times10^{-6}T^{2} + 802.200T^{-1}$

$\Delta Gf° = -490.498 - 14.910\times10^{-3}T\ln T + 2.681\times10^{-6}T^{2} + 401.100T^{-1} + 226.098\times10^{-3}T$

2000-3000 K: $\Delta Hf° = -484.484 + 9.915\times10^{-3}T - 1.359\times10^{-6}T^{2} - 1829.400T^{-1}$

$\Delta Gf° = -484.484 - 9.915\times10^{-3}T\ln T + 1.359\times10^{-6}T^{2} - 914.700T^{-1} + 188.099\times10^{-3}T$

Source: Data from JANAF (51) who estimated all except enthalpy of formation at 298 K.

$(WO_3)_4(g)$

Tetrameric Tungsten Trioxide (ideal gas)

[Formation: $4W(c) + 6O_2(g) = (WO_3)_4(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	73.894	144.635	144.635	0	-670.200	-616.356	451.795
300	74.038	145.093	144.636	.137	-670.185	-616.017	448.762
400	79.917	167.276	147.621	7.862	-669.084	-598.114	326.790
500	83.380	185.513	153.431	16.041	-667.715	-580.529	253.746
600	85.538	200.920	160.095	24.495	-666.263	-563.242	205.158
700	86.952	214.219	166.899	33.124	-664.806	-546.172	170.520
800	87.921	225.897	173.558	41.871	-663.375	-529.341	144.607
900	88.611	236.295	179.963	50.699	-661.995	-512.650	124.487
1000	89.118	245.658	186.071	59.587	-660.649	-496.127	108.427
1100	89.500	254.171	191.882	68.518	-659.364	-479.702	95.307
1200	89.794	261.972	197.402	77.484	-658.134	-463.451	84.405
1300	90.026	269.168	202.649	86.475	-656.955	-447.252	75.189
1400	90.212	275.847	207.641	95.488	-655.842	-431.127	67.301
1500	90.363	282.076	212.398	104.517	-654.777	-415.134	60.484
1600	90.487	287.912	216.938	113.559	-653.777	-399.182	54.525
1700	90.591	293.401	221.276	122.613	-652.823	-383.266	49.272
1800	90.678	298.582	225.428	131.677	-651.931	-367.477	44.617
1900	90.752	303.487	229.409	140.749	-651.095	-351.687	40.453
2000	90.815	308.143	233.230	149.827	-650.319	-335.973	36.713
2100	90.870	312.576	236.904	158.911	-649.605	-320.258	33.329
2200	90.917	316.804	240.440	168.001	-648.943	-304.639	30.263
2300	90.959	320.846	243.848	177.095	-648.345	-289.034	27.464
2400	90.995	324.718	247.138	186.192	-647.806	-273.353	24.892
2500	91.028	328.434	250.316	195.294	-647.328	-257.693	22.527
2600	91.056	332.004	253.389	204.398	-646.910	-242.158	20.355
2700	91.082	335.441	256.365	213.505	-646.547	-226.656	18.346
2800	91.105	338.754	259.249	222.614	-646.240	-211.064	16.474
2900	91.125	341.952	262.046	231.726	-645.996	-195.527	14.735
3000	91.144	345.041	264.761	240.839	-645.821	-179.930	13.108

*All data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 88.061 + 1.740\times10^{-3}T - 13.055\times10^{5}T^{-2}$

$H°- H°_{298} = 88.061\times10^{-3}T + 0.870\times10^{-6}T^{2} + 13.055\times10^{2}T^{-1} - 30.711$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -679.451 + 21.421\times10^{-3}T - 3.632\times10^{-6}T^{2} + 950.300T^{-1}$

$\Delta Gf° = -679.451 - 21.421\times10^{-3}T\ln T + 3.632\times10^{-6}T^{2} + 475.150T^{-1} + 327.244\times10^{-3}T$

2000-3000 K: $\Delta Hf° = -671.433 + 14.761\times10^{-3}T - 1.868\times10^{-6}T^{2} - 2558.500T^{-1}$

$\Delta Gf° = -671.433 - 14.761\times10^{-3}T\ln T + 1.868\times10^{-6}T^{2} - 1279.250T^{-1} + 276.579\times10^{-3}T$

Source: Data from JANAF (51) who estimated all except enthalpy of formation at 298 K.

$W_3O_8(g)$

Tritungsten Octaoxide (ideal gas)

[Formation: $3W(c) + 4O_2(g) = W_3O_8(g)$]

T, K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	49.301	118.036	118.036	0	-408.700	-378.472	277.424
300	49.398	118.341	118.038	.091	-408.694	-378.282	275.574
400	53.445	133.157	120.029	5.251	-408.147	-368.218	201.182
500	55.875	145.366	123.912	10.727	-407.413	-358.319	156.619
600	57.403	155.699	128.371	16.397	-406.617	-348.586	126.971
700	58.409	164.628	132.928	22.190	-405.814	-338.967	105.829
800	59.101	172.475	137.390	28.068	-405.024	-329.484	90.010
900	59.594	179.466	141.684	34.004	-404.267	-320.072	77.723
1000	59.956	185.765	145.783	39.982	-403.532	-310.757	67.915
1100	60.230	191.493	149.682	45.992	-402.837	-301.486	59.899
1200	60.442	196.743	153.388	52.026	-402.181	-292.322	53.238
1300	60.608	201.588	156.912	58.079	-401.559	-283.176	47.606
1400	60.741	206.084	160.265	64.147	-400.984	-274.063	42.783
1500	60.850	210.279	163.461	70.227	-400.442	-265.033	38.615
1600	60.939	214.209	166.512	76.316	-399.946	-256.015	34.970
1700	61.013	217.906	169.427	82.414	-399.482	-247.009	31.755
1800	61.076	221.395	172.218	88.518	-399.063	-238.084	28.907
1900	61.129	224.699	174.894	94.629	-398.682	-229.143	26.357
2000	61.175	227.835	177.463	100.744	-398.344	-220.246	24.067
2100	61.214	230.821	179.933	106.864	-398.049	-211.336	21.994
2200	61.248	233.670	182.312	112.987	-397.792	-202.489	20.115
2300	61.278	236.393	184.605	119.113	-397.580	-193.641	18.400
2400	61.304	239.001	186.817	125.242	-397.409	-184.723	16.821
2500	61.327	241.504	188.954	131.374	-397.282	-175.812	15.369
2600	61.348	243.910	191.022	137.508	-397.197	-166.988	14.036
2700	61.366	246.226	193.025	143.643	-397.152	-158.180	12.804
2800	61.383	248.458	194.965	149.781	-397.145	-149.295	11.653
2900	61.397	250.612	196.846	155.920	-397.184	-140.441	10.584
3000	61.411	252.694	198.674	162.060	-397.272	-131.538	9.582

*All data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 59.126 + 1.254\times10^{-3}T - 9.067\times10^{5}T^{-2}$

$H°- H°_{298} = 59.126\times10^{-3}T + 0.627\times10^{-6}T^{2} + 9.067\times10^{2}T^{-1} - 20.725$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -414.506 + 12.761\times10^{-3}T - 2.498\times10^{-6}T^{2} + 662.900T^{-1}$

$\Delta Gf° = -414.506 - 12.761\times10^{-3}T\ln T + 2.498\times10^{-6}T^{2} + 331.450T^{-1} + 189.091\times10^{-3}T$

2000-3000 K: $\Delta Hf° = -409.160 + 8.321\times10^{-3}T - 1.322\times10^{-6}T^{2} - 1676.300T^{-1}$

$\Delta Gf° = -409.160 - 8.321\times10^{-3}T\ln T + 1.322\times10^{-6}T^{2} - 838.150T^{-1} + 155.315\times10^{-3}T$

Source: Data from JANAF (51) who estimated all except enthalpy of formation at 298 K.

Xe(g)

Xenon

T, K	cal/mol•K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	4.968	40.530	40.530	0
300	4.968	40.560	40.530	.009
400	4.968	41.989	40.724	.506
500	4.968	43.098	41.092	1.003
600	4.968	44.004	41.504	1.500
700	4.968	44.770	41.919	1.996
800	4.968	45.433	42.317	2.493
900	4.968	46.018	42.696	2.990
1000	4.968	46.542	43.055	3.487
1100	4.968	47.015	43.393	3.984
1200	4.968	47.447	43.714	4.480
1300	4.968	47.845	44.017	4.977
1400	4.968	48.213	44.303	5.474
1500	4.968	48.556	44.575	5.971
1600	4.968	48.877	44.834	6.468
1700	4.968	49.178	45.082	6.964
1800	4.968	49.462	45.317	7.461
1900	4.968	49.730	45.542	7.958
2000	4.968	49.985	45.757	8.455
2100	4.968	50.227	45.964	8.952
2200	4.968	50.459	46.164	9.448
2300	4.968	50.679	46.355	9.945
2400	4.968	50.891	46.540	10.442
2500	4.968	51.094	46.718	10.939
2600	4.968	51.289	46.891	11.436
2700	4.968	51.476	47.057	11.932
2800	4.968	51.657	47.218	12.429
2900	4.968	51.831	47.374	12.926
3000	4.968	51.999	47.525	13.423

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp^\circ = 4.968$

$H^\circ - H^\circ_{298} = 4.968 \times 10^{-3} T - 1.481$

Source: Data from JANAF (52).

Y(c,1)

Yttrium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.340	10.620	10.620	0
300	6.340	10.660	10.620	.012
400	6.490	12.500	10.868	.653
500	6.650	13.970	11.350	1.310
600	6.820	15.200	11.895	1.983
700	7.000	16.260	12.440	2.674
800	7.180	17.210	12.981	3.383
900	7.360	18.060	13.493	4.110
1000	7.530	18.850	13.995	4.855
1100	7.710	19.570	14.464	5.617
1200	7.900	20.250	14.918	6.398
1300	8.070	20.890	15.355	7.196
1400	8.250	21.500	15.777	8.012
1500	8.430	22.070	16.172	8.847
1600	8.610	22.620	16.558	9.699
1700	8.830	23.150	16.934	10.568
1752	8.950	23.420	17.123	11.031
1752	8.360	24.100	17.123	12.224
1799	8.360	24.320	17.305	12.617
1799	10.300	25.830	17.305	15.341
1800	10.300	25.840	17.312	15.351
1900	10.300	26.400	17.778	16.381
2000*	10.300	26.920	18.215	17.411
2100	10.300	27.430	18.649	18.441
2200	10.300	27.910	19.060	19.471
2300	10.300	28.360	19.447	20.501
2400	10.300	28.800	19.829	21.531
2500	10.300	29.220	20.196	22.561

*Data above 1900 K extrapolated.

Phase changes: 1752 K, α - β transition point of Y; ΔH° = 1.193 kcal/mol.
1799 K, melting point of Y; ΔH° = 2.724 kcal/mol.
3611 K, boiling point of Y; ΔH° = 86.8 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1752 K: $Cp^\circ = 5.718 + 1.810\times10^{-3}T + 0.073\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.718\times10^{-3}T + 0.905\times10^{-6}T^2 - 0.073\times10^{2}T^{-1} - 1.761$

1752-1799 K: $Cp^\circ = 8.360$

$H^\circ - H^\circ_{298} = 8.360\times10^{-3}T - 2.423$

1799-2500 K: $Cp^\circ = 10.300$

$H^\circ - H^\circ_{298} = 10.300\times10^{-3}T - 3.189$

Source: Data from Hultgren (99) who extrapolated above 1900 K by assuming constant heat capacity.

Y(g)

Yttrium (ideal monatomic gas)

[Formation: Y(c,l) = Y(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	6.181	42.869	42.869	0	100.700	91.085	-66.766
300	6.181	42.907	42.869	.012	100.700	91.026	-66.311
400	6.045	44.672	43.110	.625	100.672	87.803	-47.973
500	5.826	45.997	43.561	1.218	100.608	84.595	-36.976
600	5.638	47.042	44.057	1.791	100.508	81.403	-29.651
700	5.494	47.900	44.547	2.347	100.373	78.225	-24.423
800	5.388	48.626	45.012	2.891	100.208	75.075	-20.509
900	5.308	49.256	45.449	3.426	100.016	71.940	-17.469
1000	5.248	49.812	45.859	3.953	99.798	68.836	-15.044
1100	5.203	50.310	46.241	4.476	99.559	65.745	-13.062
1200	5.169	50.761	46.599	4.994	99.296	62.683	-11.416
1300	5.143	51.174	46.936	5.510	99.014	59.645	-10.027
1400	5.127	51.554	47.252	6.023	98.711	56.635	-8.841
1500	5.119	51.908	47.551	6.535	98.388	53.631	-7.814
1600	5.119	52.238	47.834	7.047	98.048	50.659	-6.920
1700	5.130	52.549	48.103	7.559	97.691	47.713	-6.134
1752	5.141	52.703	48.235	7.827	97.496	46.191	-5.762
1752	5.141	52.703	48.235	7.827	96.303	46.191	-5.762
1799	5.152	52.839	48.354	8.069	96.152	44.842	-5.448
1799	5.152	52.839	48.354	8.069	93.428	44.842	-5.448
1800	5.152	52.842	48.356	8.074	93.423	44.819	-5.442
1900	5.187	53.122	48.601	8.590	92.909	42.137	-4.847
2000	5.235	53.389	48.833	9.111	92.400	39.462	-4.312
2100	5.298	53.646	49.056	9.638	91.897	36.843	-3.834
2200	5.377	53.894	49.270	10.172	91.401	34.236	-3.401
2300	5.472	54.135	49.477	10.714	90.913	31.630	-3.006
2400	5.584	54.370	49.675	11.267	90.436	29.068	-2.647
2500	5.713	54.601	49.869	11.831	89.970	26.517	-2.318

Phase changes: 1752 K, α - β transition point of Y; $\Delta H° = 1.193$ kcal/mol.
1799 K, melting point of Y; $\Delta H° = 2.724$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 5.510 - 0.178\times10^{-3}T + 0.644\times10^{5}T^{-2}$

$H°- H°_{298} = 5.510\times10^{-3}T - 0.089\times10^{-6}T^{2} - 0.644\times10^{2}T^{-1} - 1.419$

Formation equations (kcal/mol):

298.15-1752 K: $\Delta Hf° = 101.042 - 0.208\times10^{-3}T - 0.994\times10^{-6}T^{2} - 57.100T^{-1}$

$\Delta Gf° = 101.042 + 0.208\times10^{-3}T\ln T + 0.994\times10^{-6}T^{2} - 28.550T^{-1} - 34.556\times10^{-3}T$

1752-1799 K: $\Delta Hf° = 101.704 - 2.850\times10^{-3}T - 0.089\times10^{-6}T^{2} - 64.400T^{-1}$

$\Delta Gf° = 101.704 + 2.850\times10^{-3}T\ln T + 0.089\times10^{-6}T^{2} - 32.200T^{-1} - 53.079\times10^{-3}T$

1799-2500 K: $\Delta Hf° = 102.470 - 4.790\times10^{-3}T - 0.089\times10^{-6}T^{2} - 64.400T^{-1}$

$\Delta Gf° = 102.470 + 4.790\times10^{-3}T\ln T + 0.089\times10^{-6}T^{2} - 32.200T^{-1} - 68.045\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (238). All other data from Hilsenrath (94).

$Y_2O_3(c)$

Diyttrium Trioxide, Yttrium Sesquioxide

[Formation: $2Y(c,l) + 1.5O_2(g) = Y_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.500	23.690	23.690	0	-455.380	-434.194	318.269
300	24.557	23.842	23.692	.045	-455.378	-434.063	316.211
400	26.865	31.264	24.687	2.631	-455.139	-426.991	233.294
500	28.195	37.413	26.635	5.389	-454.792	-419.988	183.574
600	29.061	42.636	28.878	8.255	-454.405	-413.059	150.455
700	29.641	47.162	31.173	11.192	-454.017	-406.205	126.821
800	30.024	51.147	33.427	14.176	-453.648	-399.397	109.109
900	30.268	54.698	35.596	17.192	-453.307	-392.646	95.346
1000	30.418	57.896	37.669	20.227	-453.002	-385.913	84.340
1100	30.510	60.800	39.642	23.274	-452.738	-379.230	75.345
1200	30.578	63.457	41.517	26.328	-452.518	-372.556	67.851
1300	30.655	65.908	43.300	29.390	-452.336	-365.897	61.512
1330	30.684	66.608	43.819	30.310	-452.289	-363.903	59.797
1330	31.500	66.841	43.819	30.620	-451.979	-363.903	59.797
1400	31.500	68.457	45.011	32.825	-451.828	-359.257	56.082
1500	31.500	70.630	46.647	35.975	-451.654	-352.669	51.383
1600	31.500	72.663	48.210	39.125	-451.523	-346.074	47.271
1700	31.500	74.573	49.705	42.275	-451.434	-339.475	43.642
1752	31.500	75.522	50.457	43.913	-451.414	-336.044	41.919
1752	31.500	75.522	50.457	43.913	-453.800	-336.044	41.919
1799	31.500	76.355	51.123	45.393	-453.732	-332.900	40.442
1799	31.500	76.355	51.123	45.393	-459.180	-332.900	40.442
1800	31.500	76.373	51.137	45.425	-459.182	-332.822	40.410
1900	31.500	78.076	52.510	48.575	-459.433	-325.784	37.473
2000	31.500	79.692	53.830	51.725	-459.691	-318.777	34.834

Phase changes: 1330 K, α - β transition point of Y_2O_3; ΔH° = 0.310 kcal/mol.
1752 K, α - β transition point of Y; ΔH° = 1.193 kcal/mol.
1799 K, melting point of Y; ΔH° = 2.724 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1330 K: $Cp° = 29.421 + 1.414\times10^{-3}T - 4.749\times10^{5}T^{-2}$

$H°- H°_{298} = 29.421\times10^{-3}T + 0.707\times10^{-6}T^2 + 4.749\times10^{2}T^{-1} - 10.428$

1330-2000 K: $Cp° = 31.500$

$H°- H°_{298} = 31.500\times10^{-3}T - 11.275$

Formation equations (kcal/mol):

298.15-1330 K: $\Delta Hf° = -458.758 + 7.140\times10^{-3}T - 1.858\times10^{-6}T^2 + 421.700T^{-1}$

$\Delta Gf° = -458.758 - 7.140\times10^{-3}T\ln T + 1.858\times10^{-6}T^2 + 210.850T^{-1} + 120.143\times10^{-3}T$

1330-1752 K: $\Delta Hf° = -459.605 + 9.219\times10^{-3}T - 2.565\times10^{-6}T^2 - 53.200T^{-1}$

$\Delta Gf° = -459.605 - 9.219\times10^{-3}T\ln T + 2.565\times10^{-6}T^2 - 26.600T^{-1} + 134.928\times10^{-3}T$

1752-1799 K: $\Delta Hf° = -458.281 + 3.935\times10^{-3}T - 0.754\times10^{-6}T^2 - 67.800T^{-1}$

$\Delta Gf° = -458.281 - 3.935\times10^{-3}T\ln T + 0.754\times10^{-6}T^2 - 33.900T^{-1} + 97.882\times10^{-3}T$

1799-2000 K: $\Delta Hf° = -456.749 + 0.055\times10^{-3}T - 0.754\times10^{-6}T^2 - 67.800T^{-1}$

$\Delta Gf° = -456.749 - 0.055\times10^{-3}T\ln T + 0.754\times10^{-6}T^2 - 33.900T^{-1} + 67.950\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (238). Low-temperature heat capacities and entropy at 298 K from Goldstein (80). High-temperature data based on Pankratz (179).

Yb(c,l,g)

Ytterbium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.390	14.300	14.300	0
300	6.390	14.340	14.300	.012
400	6.600	16.200	14.553	.659
500	7.410	17.750	15.046	1.352
553	8.290	18.540	15.343	1.768
600	7.130	19.120	15.617	2.102
700	7.250	20.230	16.201	2.820
800	7.370	21.200	16.761	3.551
900	7.500	22.080	17.308	4.295
1000	7.640	22.870	17.819	5.051
1033	7.660	23.120	17.987	5.305
1033	8.640	23.530	17.987	5.723
1097	8.640	24.050	18.330	6.276
1097	8.790	25.720	18.330	8.106
1100	8.790	25.740	18.348	8.131
1200	8.790	26.500	18.992	9.010
1300	8.790	27.210	19.603	9.889
1400	8.790	27.860	20.169	10.768
1467	8.790	28.270	20.530	11.357
1467	4.968	49.267	20.530	42.157
1500	4.968	49.378	21.164	42.321
1600	4.968	49.698	22.937	42.818
1700	4.969	50.000	24.521	43.314
1800	4.969	50.284	25.945	43.811
1900	4.971	50.552	27.232	44.308
2000	4.973	50.807	28.404	44.805

Phase changes: 553 K, second order transition of Yb; ΔH° = 0 kcal/mol.
1033 K, $\alpha - \beta$ transition of Yb; ΔH° = 0.418 kcal/mol.
1097 K, melting point of Yb; ΔH° = 1.830 kcal/mol.
1467 K, boiling point of Yb; ΔH° = 30.800 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-553 K:
$$C_p^\circ = 1.024 + 11.404\times10^{-3}T + 1.747\times10^{5}T^{-2}$$
$$H^\circ - H^\circ_{298} = 1.024\times10^{-3}T + 5.702\times10^{-6}T^2 - 1.747\times10^{2}T^{-1} - 0.226$$

553-1033 K:
$$C_p^\circ = 6.228 + 1.388\times10^{-3}T + 0.227\times10^{5}T^{-2}$$
$$H^\circ - H^\circ_{298} = 6.228\times10^{-3}T + 0.694\times10^{-6}T^2 - 0.227\times10^{2}T^{-1} - 1.847$$

1033-1097 K:
$$C_p^\circ = 8.640$$
$$H^\circ - H^\circ_{298} = 8.640\times10^{-3}T - 3.202$$

1097-1467 K:
$$C_p^\circ = 8.786$$
$$H^\circ - H^\circ_{298} = 8.786\times10^{-3}T - 1.532$$

1467-2000 K:
$$C_p^\circ = 4.968$$
$$H^\circ - H^\circ_{298} = 4.968\times10^{-3}T + 34.869$$

Sources: Data for Yb(c,l) from Hultgren (99). Data for Yb(g) from Feber (58).

Yb(g)

Ytterbium (ideal monatomic gas)

[Formation: Yb(c,l,g) = Yb(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	4.968	41.352	41.352	0	36.350	28.284	-20.733
300	4.968	41.382	41.352	.009	36.347	28.234	-20.568
400	4.968	42.812	41.547	.506	36.197	25.552	-13.961
500	4.968	43.920	41.914	1.003	36.001	22.916	-10.016
553	4.968	44.421	42.131	1.267	35.848	21.536	-8.511
600	4.968	44.826	42.326	1.500	35.748	20.324	-7.403
700	4.968	45.592	42.741	1.996	35.526	17.773	-5.549
800	4.968	46.255	43.139	2.493	35.292	15.248	-4.166
900	4.968	46.840	43.518	2.990	35.045	12.761	-3.099
1000	4.968	47.364	43.877	3.487	34.786	10.292	-2.249
1033	4.968	47.525	43.991	3.651	34.696	9.488	-2.007
1033	4.968	47.525	43.991	3.651	34.278	9.488	-2.007
1097	4.968	47.823	44.205	3.969	34.043	7.966	-1.587
1097	4.968	47.823	44.205	3.969	32.213	7.966	-1.587
1100	4.968	47.837	44.215	3.984	32.203	7.896	-1.569
1200	4.968	48.269	44.536	4.480	31.820	5.697	-1.038
1300	4.968	48.667	44.839	4.977	31.438	3.544	-.596
1400	4.968	49.035	45.125	5.474	31.056	1.411	-.220
1467	4.968	49.267	45.309	5.807	30.800	0	0
1467	4.968	49.267	45.309	5.807	0	0	0
1500	4.968	49.378	45.397	5.971	0	0	0
1600	4.968	49.698	45.656	6.468	0	0	0
1700	4.969	50.000	45.904	6.964	0	0	0
1800	4.969	50.284	46.139	7.461	0	0	0
1900	4.971	50.552	46.364	7.958	0	0	0
2000	4.973	50.807	46.579	8.455	0	0	0

Phase changes: 553 K, second order transition of Yb; $\Delta H° = 0$ kcal/mol.
1033 K, α - β transition point of Yb; $\Delta H° = 0.418$ kcal/mol.
1097 K, melting point of Yb; $\Delta H° = 1.830$ kcal/mol.
1467 K, boiling point of Yb; $\Delta H° = 30.800$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.968$

$H°- H°_{298} = 4.968\times10^{-3}T - 1.481$

Formation equations (kcal/mol):

298.15-553 K: $\Delta Hf° = 35.095 + 3.944\times10^{-3}T - 5.702\times10^{-6}T^2 + 174.700T^{-1}$

$\Delta Gf° = 35.095 - 3.944\times10^{-3}T\ln T + 5.702\times10^{-6}T^2 + 87.350T^{-1} - 3.054\times10^{-3}T$

553-1033 K: $\Delta Hf° = 36.716 - 1.260\times10^{-3}T - 0.694\times10^{-6}T^2 + 22.700T^{-1}$

$\Delta Gf° = 36.716 + 1.260\times10^{-3}T\ln T + 0.694\times10^{-6}T^2 + 11.350T^{-1} - 35.833\times10^{-3}T$

1033-1097 K: $\Delta Hf° = 38.071 - 3.672\times10^{-3}T$

$\Delta Gf° = 38.071 + 3.672\times10^{-3}T\ln T - 53.157\times10^{-3}T$

1097-1467 K: $\Delta Hf° = 36.401 - 3.818\times10^{-3}T$

$\Delta Gf° = 36.401 + 3.818\times10^{-3}T\ln T - 52.657\times10^{-3}T$

1467-2000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Sources: Enthalpy of formation at 298 K from Hultgren (99). All other data from Feber (58).

$Yb_2O_3(c)$

Diytterbium Trioxide, Ytterbium Sesquioxide

[Formation: $2Yb(c,l,g) + 1.5O_2(g) = Yb_2O_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	27.570	31.800	31.800	0	-433.680	-412.718	302.526
300	27.620	31.971	31.801	.051	-433.672	-412.588	300.566
400	29.381	40.176	32.906	2.908	-433.174	-405.631	221.624
500	30.336	46.846	35.050	5.898	-432.667	-398.799	174.313
553	30.627	49.920	36.328	7.516	-432.476	-395.219	156.191
600	30.885	52.429	37.492	8.962	-432.235	-392.062	142.807
700	31.207	57.217	39.977	12.068	-431.733	-385.402	120.326
800	31.389	61.397	42.398	15.199	-431.260	-378.826	103.489
900	31.480	65.100	44.719	18.343	-430.826	-372.291	90.403
1000	31.516	68.419	46.926	21.493	-430.428	-365.822	79.949
1033	31.519	69.442	47.629	22.533	-430.309	-363.688	76.944
1033	31.519	69.442	47.629	22.533	-431.145	-363.688	76.944
1097	31.526	71.337	48.957	24.550	-431.041	-359.500	71.621
1097	31.526	71.337	48.957	24.550	-434.701	-359.500	71.621
1100	31.526	71.423	49.018	24.645	-434.695	-359.298	71.385
1200	31.534	74.167	51.002	27.798	-434.572	-352.461	64.191
1300	31.561	76.692	52.883	30.952	-434.460	-345.608	58.101
1365	31.599	78.232	54.053	33.005	-434.391	-341.170	54.624
1365	32.150	78.342	54.053	33.155	-434.241	-341.170	54.624
1400	32.150	79.156	54.670	34.280	-434.185	-338.785	52.886
1467	32.150	80.659	55.823	36.434	-434.083	-334.222	49.791
1467	32.150	80.659	55.823	36.434	-495.683	-334.222	49.791
1500	32.150	81.374	56.377	37.495	-495.382	-330.589	48.166
1600	32.150	83.449	58.005	40.710	-494.476	-319.635	43.660
1700	32.150	85.398	59.560	43.925	-493.576	-308.730	39.689
1800	32.150	87.236	61.047	47.140	-492.687	-297.882	36.167
1900	32.150	88.974	62.471	50.355	-491.807	-287.087	33.022
2000	32.150	90.623	63.838	53.570	-490.934	-276.334	30.196

Phase changes: 553 K, second order transition point of Yb; $\Delta H° = 0$ kcal/mol.
1033 K, α - β transition point of Yb; $\Delta H° = 0.418$ kcal/mol.
1097 K, melting point of Yb; $\Delta H° = 1.830$ kcal/mol.
1365 K, α - β transition point of Yb_2O_3; $\Delta H° = 0.150$ kcal/mol.
1467 K, boiling point of Yb; $\Delta H° = 30.800$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1365 K: $Cp° = 31.817 + 0.062\times10^{-3}T - 3.792\times10^{5}T^{-2}$

$H°- H°_{298} = 31.817\times10^{-3}T + 0.031\times10^{-6}T^{2} + 3.792\times10^{2}T^{-1} - 10.761$

1365-2000 K: $Cp° = 32.150$

$H°- H°_{298} = 32.150\times10^{-3}T - 10.730$

Yb_2O_3(c) - Continued

Formation equations (kcal/mol):

298.15-553 K: $\Delta Hf^\circ = -440.460 + 18.924\times10^{-3}T - 12.128\times10^{-6}T^2 + 660.800T^{-1}$

$\Delta Gf^\circ = -440.460 - 18.924\times10^{-3}T\ln T + 12.128\times10^{-6}T^2 + 330.400T^{-1} + 193.538\times10^{-3}T$

553-1033 K: $\Delta Hf^\circ = -437.218 + 8.516\times10^{-3}T - 2.112\times10^{-6}T^2 + 356.800T^{-1}$

$\Delta Gf^\circ = -437.218 - 8.516\times10^{-3}T\ln T + 2.112\times10^{-6}T^2 + 178.400T^{-1} + 127.980\times10^{-3}T$

1033-1097 K: $\Delta Hf^\circ = -434.508 + 3.692\times10^{-3}T - 0.723\times10^{-6}T^2 + 311.400T^{-1}$

$\Delta Gf^\circ = -434.508 - 3.692\times10^{-3}T\ln T + 0.723\times10^{-6}T^2 + 155.700T^{-1} + 93.332\times10^{-3}T$

1097-1365 K: $\Delta Hf^\circ = -437.848 + 3.400\times10^{-3}T - 0.723\times10^{-6}T^2 + 311.400T^{-1}$

$\Delta Gf^\circ = -437.848 - 3.400\times10^{-3}T\ln T + 0.723\times10^{-6}T^2 + 155.700T^{-1} + 94.333\times10^{-3}T$

1365-1467 K: $\Delta Hf^\circ = -437.817 + 3.733\times10^{-3}T - 0.754\times10^{-6}T^2 - 67.800T^{-1}$

$\Delta Gf^\circ = -437.817 - 3.733\times10^{-3}T\ln T + 0.754\times10^{-6}T^2 - 33.900T^{-1} + 96.773\times10^{-3}T$

1467-2000 K: $\Delta Hf^\circ = -510.619 + 11.369\times10^{-3}T - 0.754\times10^{-6}T^2 - 67.800T^{-1}$

$\Delta Gf^\circ = -510.619 - 11.369\times10^{-3}T\ln T + 0.754\times10^{-6}T^2 - 33.900T^{-1} + 202.074\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (192). Low-temperature heat capacities and entropy at 298 K from Justice (110). High-temperature data based on Pankratz (178).

Zn(c,l,g)

Zinc

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.070	9.950	9.950	0
300	6.074	9.988	9.951	.011
400	6.285	11.765	10.193	.629
500	6.520	13.191	10.653	1.269
600	6.809	14.405	11.180	1.935
692.73	7.069	15.400	11.676	2.580
692.73	7.500	17.927	11.676	4.330
700	7.500	18.006	11.742	4.385
800	7.500	19.008	12.589	5.135
900	7.500	19.891	13.352	5.885
1000	7.500	20.681	14.046	6.635
1100	7.500	21.396	14.682	7.385
1180	7.500	21.925	15.158	7.985
1180	4.968	45.285	15.158	35.550
1200	4.968	45.368	15.660	35.650
1300	4.968	45.765	17.960	36.147
1400	4.968	46.134	19.960	36.644
1500	4.968	46.476	21.715	37.141
1600	4.968	46.797	23.273	37.638
1700	4.968	47.098	24.666	38.135
1800	4.968	47.382	25.920	38.632
1900	4.968	47.651	27.057	39.129
2000	4.968	47.905	28.092	39.626

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.
1180 K, boiling point of Zn; ΔH° = 27.565 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-692.73 K: $Cp^\circ = 5.099 + 2.784\times10^{-3}T + 0.126\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.099\times10^{-3}T + 1.392\times10^{-6}T^2 - 0.126\times10^{2}T^{-1} - 1.602$

692.73-1180 K: $Cp^\circ = 7.500$

$H^\circ - H^\circ_{298} = 7.500\times10^{-3}T - 0.865$

1180-2000 K: $Cp^\circ = 4.968$

$H^\circ - H^\circ_{298} = 4.968\times10^{-3}T + 29.688$

Source: Data from Hultgren (99).

Zn(g)

Zinc (ideal monatomic gas)

[Formation: Zn(c,l,g) = Zn(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^{\circ}_{298})/T$	$H°-H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15	4.968	38.451	38.451	0	31.170	22.672	-16.619
300	4.968	38.481	38.451	.009	31.168	22.620	-16.479
400	4.968	39.911	38.646	.506	31.047	19.789	-10.812
500	4.968	41.019	39.013	1.003	30.904	16.990	-7.426
600	4.968	41.925	39.425	1.500	30.735	14.223	-5.181
692.73	4.968	42.639	39.810	1.960	30.550	11.681	-3.685
692.73	4.968	42.639	39.810	1.960	28.800	11.681	-3.685
700	4.968	42.691	39.840	1.996	28.781	11.501	-3.591
800	4.968	43.354	40.238	2.493	28.528	9.051	-2.473
900	4.968	43.939	40.617	2.990	28.275	6.632	-1.610
1000	4.968	44.463	40.976	3.487	28.022	4.240	-.927
1100	4.968	44.936	41.314	3.984	27.769	1.875	-.373
1180	4.968	45.285	41.572	4.381	27.565	0	0
1180	4.968	45.285	41.572	4.381	0	0	0
1200	4.968	45.368	41.635	4.480	0	0	0
1300	4.968	45.765	41.937	4.977	0	0	0
1400	4.968	46.134	42.224	5.474	0	0	0
1500	4.968	46.476	42.495	5.971	0	0	0
1600	4.968	46.797	42.755	6.468	0	0	0
1700	4.968	47.098	43.002	6.964	0	0	0
1800	4.968	47.382	43.237	7.461	0	0	0
1900	4.968	47.651	43.463	7.958	0	0	0
2000	4.968	47.905	43.677	8.455	0	0	0

Phase changes: 692.73 K, melting point of Zn; $\Delta H° = 1.750$ kcal/mol.
1180 K, boiling point of Zn; $\Delta H° = 27.565$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 4.968$

$H°-H^{\circ}_{298} = 4.968\times10^{-3}T - 1.481$

Formation equations (kcal/mol):

298.15-692.73 K: $\Delta Hf° = 31.291 - 0.131\times10^{-3}T - 1.392\times10^{-6}T^2 + 12.600T^{-1}$

$\Delta Gf° = 31.291 + 0.131\times10^{-3}T\ln T + 1.392\times10^{-6}T^2 + 6.300T^{-1} - 30.138\times10^{-3}T$

692.73-1180 K: $\Delta Hf° = 30.554 - 2.532\times10^{-3}T$

$\Delta Gf° = 30.554 + 2.532\times10^{-3}T\ln T - 43.801\times10^{-3}T$

1180-2000 K: $\Delta Hf° = 0$

$\Delta Gf° = 0$

Sources: Enthalpy of formation at 298 K from CODATA (36). All other data from Hilsenrath (94).

ZnO(c)

Zinc Oxide

[Formation: $Zn(c,l,g) + 0.5O_2(g) = ZnO(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.820	10.430	10.430	0	-83.762	-76.600	56.148
300	9.830	10.490	10.430	.018	-83.762	-76.555	55.769
400	10.680	13.450	10.828	1.049	-83.703	-74.159	40.518
500	11.160	15.890	11.604	2.143	-83.615	-71.784	31.376
600	11.500	17.950	12.488	3.277	-83.524	-69.422	25.287
692.73	11.760	19.627	13.340	4.355	-83.451	-67.255	21.218
692.73	11.760	19.627	13.340	4.355	-85.201	-67.255	21.218
700	11.780	19.750	13.406	4.441	-85.200	-67.067	20.939
800	12.010	21.340	14.301	5.631	-85.159	-64.480	17.615
900	12.230	22.770	15.166	6.844	-85.103	-61.900	15.031
1000	12.440	24.070	15.992	8.078	-85.032	-59.326	12.966
1100	12.640	25.260	16.776	9.332	-84.948	-56.753	11.276
1180	12.792	26.155	17.385	10.349	-84.870	-54.706	10.132
1180	12.792	26.155	17.385	10.349	-112.435	-54.706	10.132
1200	12.830	26.370	17.533	10.605	-112.364	-53.729	9.785
1300	13.020	27.400	18.248	11.898	-111.995	-48.853	8.213
1400	13.210	28.370	18.934	13.210	-111.613	-44.006	6.870
1500	13.390	29.290	19.597	14.540	-111.215	-39.196	5.711
1600	13.570	30.160	20.230	15.888	-110.802	-34.408	4.700
1700	13.750	30.990	20.841	17.254	-110.374	-29.649	3.812
1800	13.930	31.780	21.425	18.639	-109.930	-24.911	3.025
1900	14.110	32.540	21.992	20.041	-109.472	-20.203	2.324
2000	14.290	33.270	22.540	21.461	-108.999	-15.522	1.696

Phase changes: 692.73 K, melting point of Zn; $\Delta H° = 1.750$ kcal/mol.
1180 K, boiling point of Zn; $\Delta H° = 27.565$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.836 + 1.742\times10^{-3}T - 1.365\times10^{5}T^{-2}$

$H°- H°_{298} = 10.836\times10^{-3}T + 0.871\times10^{-6}T^{2} + 1.365\times10^{2}T^{-1} - 3.766$

Formation equations (kcal/mol):

298.15-692.73 K: $\Delta Hf° = -84.750 + 2.122\times10^{-3}T - 0.773\times^{-6}T^{2} + 126.500T^{-1}$

$\Delta Gf° = -84.750 - 2.122\times10^{-3}T\ln T + 0.773\times^{-6}T^{2} + 63.250T^{-1} + 38.486\times10^{-3}T$

692.73-1180 K: $\Delta Hf° = -85.487 - 0.279\times10^{-3}T + 0.620\times^{-6}T^{2} + 113.900T^{-1}$

$\Delta Gf° = -85.487 + 0.279\times10^{-3}T\ln T - 0.620\times10^{-6}T^{2} + 56.950T^{-1} + 24.822\times10^{-3}T$

1180-2000 K: $\Delta Hf° = -116.040 + 2.253\times10^{-3}T + 0.620\times10^{-6}T^{2} + 113.900T^{-1}$

$\Delta Gf° = -116.040 - 2.253\times10^{-3}T\ln T - 0.620\times10^{-6}T^{2} + 56.950T^{-1} + 68.624\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (36). Heat capacity at 298 K and high-temperature data from Mills (157).

Zr(c,l)

Zirconium

T, K	cal/mol·K			$H^\circ - H^\circ_{298}$,
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	kcal/mol
298.15	6.186	9.320	9.320	0
300	6.194	9.358	9.321	.011
400	6.546	11.195	9.568	.651
500	6.800	12.684	10.048	1.318
600	7.027	13.944	10.594	2.010
700	7.240	15.043	11.153	2.723
800	7.446	16.023	11.701	3.458
900	7.647	16.912	12.232	4.212
1000	7.846	17.728	12.741	4.987
1100	8.044	18.485	13.230	5.781
1136	8.114	18.745	13.400	6.072
1136	6.683	19.582	13.400	7.023
1200	6.786	19.952	13.740	7.454
1300	6.946	20.501	14.239	8.141
1400	7.107	21.022	14.706	8.843
1500	7.268	21.518	15.143	9.562
1600	7.428	21.992	15.556	10.297
1700	7.589	22.447	15.948	11.048
1800	7.749	22.885	16.321	11.815
1900	7.910	23.308	16.677	12.598
2000	8.071	23.718	17.020	13.397
2100	8.231	24.116	17.348	14.212
2125	8.271	24.213	17.428	14.418
2125*	8.000	26.566	17.428	19.418
2200	8.000	26.843	17.744	20.018
2300	8.000	27.199	18.148	20.818
2400	8.000	27.540	18.533	21.618
2500	8.000	27.866	18.899	22.418
2600	8.000	28.180	19.250	23.218
2700	8.000	28.482	19.586	24.018
2800	8.000	28.773	19.909	24.818
2900	8.000	29.054	20.220	25.618
3000	8.000	29.325	20.519	26.418

*Data for Zr(l) estimated.

Phase changes: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.
2125 K, melting point of Zr; ΔH° = 5.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1136 K: $Cp^\circ = 5.993 + 1.884\times10^{-3}T - 0.329\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 5.993\times10^{-3}T + 0.942\times10^{-6}T^2 + 0.329\times10^{2}T^{-1} - 1.981$

1136-2125 K: $Cp^\circ = 4.824 + 1.622\times10^{-3}T + 0.216\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 4.824\times10^{-3}T + 0.811\times10^{-6}T^2 - 0.216\times10^{2}T^{-1} + 0.515$

2125-3000 K: $Cp^\circ = 8.000$

$H^\circ - H^\circ_{298} = 8.000\times10^{-3}T + 2.418$

Sources: Entropy at 298 K from Wagman (238). Low-temperature heat capacities from Todd (220). High-temperature data for Zr(c) based on Douglas (50) and Skinner (203). Data for Zr(l) estimated.

Zr(g)

Zirconium (ideal monatomic gas)

[Formation: Zr(c,l) = Zr(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	6.367	43.315	43.315	0	148.300	138.164	-101.276
300	6.375	43.354	43.315	.012	148.301	138.102	-100.606
400	6.612	45.229	43.569	.664	148.313	134.699	-73.595
500	6.594	46.706	44.054	1.326	148.308	131.297	-57.389
600	6.464	47.897	44.599	1.979	148.269	127.897	-46.586
700	6.315	48.882	45.142	2.618	148.195	124.508	-38.873
800	6.198	49.717	45.663	3.243	148.085	121.130	-33.091
900	6.133	50.443	46.155	3.859	147.947	117.769	-28.598
1000	6.121	51.088	46.616	4.472	147.785	114.425	-25.007
1100	6.155	51.673	47.050	5.085	147.604	111.097	-22.073
1136	6.180	51.872	47.200	5.307	147.535	109.903	-21.144
1136	6.180	51.872	47.200	5.307	146.584	109.903	-21.144
1200	6.225	52.211	47.458	5.704	146.550	107.839	-19.640
1300	6.320	52.713	47.843	6.331	146.490	104.614	-17.587
1400	6.428	53.185	48.208	6.968	146.425	101.397	-15.829
1500	6.542	53.633	48.555	7.617	146.355	98.183	-14.305
1600	6.655	54.059	48.886	8.276	146.279	94.972	-12.972
1700	6.763	54.465	49.202	8.947	146.199	91.768	-11.797
1800	6.865	54.855	49.506	9.629	146.114	88.568	-10.753
1900	6.959	55.229	49.797	10.320	146.022	85.372	-9.820
2000	7.046	55.588	50.078	11.021	145.924	82.184	-8.981
2100	7.127	55.934	50.349	11.729	145.817	78.999	-8.221
2125	7.146	56.018	50.415	11.907	145.789	78.203	-8.043
2125	7.146	56.018	50.415	11.907	140.789	78.203	-8.043
2200	7.202	56.267	50.610	12.446	140.728	75.995	-7.549
2300	7.273	56.588	50.862	13.169	140.651	73.056	-6.942
2400	7.341	56.899	51.107	13.900	140.582	70.120	-6.385
2500	7.408	57.201	51.346	14.638	140.520	67.183	-5.873
2600	7.475	57.492	51.576	15.382	140.464	64.253	-5.401
2700	7.542	57.776	51.801	16.133	140.415	61.321	-4.964
2800	7.609	58.051	52.019	16.890	140.372	58.394	-4.558
2900	7.678	58.319	52.231	17.654	140.336	55.468	-4.180
3000	7.749	58.581	52.439	18.426	140.308	52.540	-3.827

Phase changes: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.
2125 K, melting point of Zr; ΔH° = 5.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:

$$Cp° = 6.180 + 0.242\times10^{-3}T + 0.104\times10^{5}T^{-2}$$

$$H°- H°_{298} = 6.180\times10^{-3}T + 0.121\times10^{-6}T^{2} - 0.104\times10^{2}T^{-1} - 1.818$$

2000-3000 K:

$$Cp° = 6.397 + 0.490\times10^{-3}T - 13.219\times10^{5}T^{-2}$$

$$H°- H°_{298} = 6.397\times10^{-3}T + 0.245\times10^{-6}T^{2} + 13.219\times10^{2}T^{-1} - 3.414$$

Zr(g) - Continued

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf^\circ = 148.462 + 0.187\times10^{-3}T - 0.821\times10^{-6}T^2 - 43.300T^{-1}$

$\Delta Gf^\circ = 148.462 - 0.187\times10^{-3}T\ln T + 0.821\times10^{-6}T^2 - 21.650T^{-1} - 33.476\times10^{-3}T$

1136-2000 K: $\Delta Hf^\circ = 145.966 + 1.356\times10^{-3}T - 0.690\times10^{-6}T^2 + 11.200T^{-1}$

$\Delta Gf^\circ = 145.966 - 1.356\times10^{-3}T\ln T + 0.690\times10^{-6}T^2 + 5.600T^{-1} - 22.927\times10^{-3}T$

2000-2125 K: $\Delta Hf^\circ = 144.370 + 1.573\times10^{-3}T - 0.566\times10^{-6}T^2 + 1343.500T^{-1}$

$\Delta Gf^\circ = 144.370 - 1.573\times10^{-3}T\ln T + 0.566\times10^{-6}T^2 + 671.750T^{-1} - 20.398\times10^{-3}T$

2125-3000 K: $\Delta Hf^\circ = 142.467 - 1.603\times10^{-3}T + 0.245\times10^{-6}T^2 + 1321.900T^{-1}$

$\Delta Gf^\circ = 142.467 + 1.603\times10^{-3}T\ln T - 0.245\times10^{-6}T^2 + 660.950T^{-1} - 42.109\times10^{-3}T$

Source: Data from JANAF (51).

ZrO(g)

Zirconium Oxide (ideal gas)

[Formation: $Zr(c) + 0.5O_2(g) = ZrO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.373	54.332	54.332	0	15.000	8.885	-6.513
300	7.380	54.378	54.332	.014	14.997	8.848	-6.446
400	7.754	56.553	54.625	.771	14.759	6.833	-3.733
500	8.066	58.318	55.194	1.562	14.517	4.880	-2.133
600	8.343	59.813	55.841	2.383	14.268	2.976	-1.084
700	8.644	61.121	56.504	3.232	14.016	1.115	-.348
800	9.010	62.299	57.157	4.114	13.764	-.713	.195
900	9.450	63.385	57.789	5.036	13.524	-2.508	.609
1000	9.948	64.406	58.400	6.006	13.306	-4.277	.935
1100	10.471	65.378	58.990	7.027	13.114	-6.024	1.197
1136	10.654	65.718	59.198	7.407	13.051	-6.650	1.279
1136	10.654	65.718	59.198	7.407	12.100	-6.650	1.279
1200	10.980	66.311	59.562	8.099	12.089	-7.705	1.403
1300	11.443	67.209	60.116	9.221	12.096	-9.356	1.573
1400	11.833	68.072	60.653	10.386	12.126	-11.006	1.718
1500	12.139	68.899	61.176	11.585	12.172	-12.660	1.845
1600	12.358	69.690	61.683	12.811	12.224	-14.318	1.956
1700	12.494	70.444	62.177	14.054	12.275	-15.979	2.054
1800	12.557	71.160	62.656	15.307	12.317	-17.642	2.142
1900	12.561	71.839	63.122	16.563	12.343	-19.308	2.221
2000	12.517	72.483	63.575	17.817	12.349	-20.975	2.292

Phase change: 1136 K, α - β transition point of Zr; $\Delta H° = 0.951$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.126 + 3.818\times10^{-3}T + 0.097\times10^{5}T^{-2}$

$H°- H°_{298} = 6.126\times10^{-3}T + 1.909\times10^{-6}T^{2} - 0.097\times10^{2}T^{-1} - 1.964$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf° = 16.193 - 3.482\times10^{-3}T + 0.716\times10^{-6}T^{2} - 65.200T^{-1}$

$\Delta Gf° = 16.193 + 3.482\times10^{-3}T\ln T - 0.716\times10^{-6}T^{2} - 32.600T^{-1} - 43.771\times10^{-3}T$

1136-2000 K: $\Delta Hf° = 13.697 - 2.313\times10^{-3}T + 0.847\times10^{-6}T^{2} - 10.700T^{-1}$

$\Delta Gf° = 13.697 + 2.313\times10^{-3}T\ln T - 0.847\times10^{-6}T^{2} - 5.350T^{-1} - 33.221\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (238). All other data from JANAF (51).

$ZrO_2(c)$

Zirconium Dioxide

[Formation: $Zr(c,1) + O_2(g) = ZrO_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.430	12.040	12.040	0	-263.040	-249.240	182.696
300	13.475	12.123	12.040	.025	-263.039	-249.154	181.506
400	15.155	16.251	12.591	1.464	-262.950	-244.536	133.607
500	16.141	19.746	13.682	3.032	-262.780	-239.950	104.881
600	16.813	22.752	14.949	4.682	-262.577	-235.404	85.745
700	17.314	25.383	16.256	6.389	-262.361	-230.892	72.087
800	17.706	27.722	17.546	8.141	-262.142	-226.413	61.852
900	18.016	29.826	18.795	9.928	-261.923	-221.959	53.898
1000	18.261	31.737	19.995	11.742	-261.711	-217.530	47.541
1100	18.448	33.487	21.143	13.578	-261.508	-213.121	42.343
1136	18.496	34.082	21.544	14.243	-261.438	-211.539	40.697
1136	18.496	34.082	21.544	14.243	-262.389	-211.539	40.697
1200	18.582	35.098	22.240	15.430	-262.177	-208.679	38.005
1300	18.668	36.589	23.287	17.293	-261.857	-204.235	34.335
1400	18.708	37.974	24.287	19.162	-261.554	-199.813	31.192
1478	18.708	38.988	25.037	20.620	-261.334	-196.380	29.038
1478	18.780	40.294	25.037	22.550	-259.404	-196.380	29.038
1500	18.780	40.572	25.263	22.963	-259.342	-195.444	28.476
1600	18.780	41.784	26.258	24.841	-259.076	-191.193	26.115
1700	18.780	42.922	27.205	26.719	-258.831	-186.957	24.035
1800	18.780	43.996	28.109	28.597	-258.608	-182.736	22.187
1900	18.780	45.011	28.972	30.475	-258.407	-178.527	20.535
2000	18.780	45.974	29.797	32.353	-258.227	-174.327	19.049
2100	18.780	46.890	30.590	34.231	-258.069	-170.134	17.706
2125	18.780	47.112	30.783	34.701	-258.033	-169.088	17.390
2125	18.780	47.112	30.783	34.701	-263.033	-169.088	17.390
2200	18.780	47.764	31.351	36.109	-262.907	-165.777	16.468
2300	18.780	48.599	32.083	37.987	-262.745	-161.366	15.333
2400	18.780	49.398	32.788	39.865	-262.588	-156.959	14.293
2500	18.780	50.165	33.468	41.743	-262.436	-152.564	13.337

Phase changes: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.
1478 K, α - β transition point of ZrO_2; ΔH° = 1.930 kcal/mol.
2125 K, melting point of Zr; ΔH° = 5.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1478 K: $Cp° = 16.759 + 1.678\times10^{-3}T - 3.404\times10^{5}T^{-2}$

$H°- H°_{298} = 16.759\times10^{-3}T + 0.839\times10^{-6}T^{2} + 3.404\times10^{2}T^{-1} - 6.213$

1478-2500 K: $Cp° = 18.780$

$H°- H°_{298} = 18.780\times10^{-3}T - 5.207$

ZrO_2(c) - Continued

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf^\circ = -264.920 + 3.536\times10^{-3}T - 0.606\times10^{-6}T^2 + 262.300T^{-1}$

$\Delta Gf^\circ = -264.920 - 3.536\times10^{-3}T\ln T + 0.606\times10^{-6}T^2 + 131.150T^{-1} + 71.082\times10^{-3}T$

1136-1478 K: $\Delta Hf^\circ = -267.416 + 4.705\times10^{-3}T - 0.475\times10^{-6}T^2 + 316.800T^{-1}$

$\Delta Gf^\circ = -267.416 - 4.705\times10^{-3}T\ln T + 0.475\times10^{-6}T^2 + 158.400T^{-1} + 81.631\times10^{-3}T$

1478-2000 K: $\Delta Hf^\circ = -266.410 + 6.726\times10^{-3}T - 1.314\times10^{-6}T^2 - 23.600T^{-1}$

$\Delta Gf^\circ = -266.410 - 6.726\times10^{-3}T\ln T + 1.314\times10^{-6}T^2 - 11.800T^{-1} + 94.538\times10^{-3}T$

2000-2125 K: $\Delta Hf^\circ = -265.074 + 5.616\times10^{-3}T - 1.020\times10^{-6}T^2 - 608.400T^{-1}$

$\Delta Gf^\circ = -265.074 - 5.616\times10^{-3}T\ln T + 1.020\times10^{-6}T^2 - 304.200T^{-1} + 86.094\times10^{-3}T$

2125-2500 K: $\Delta Hf^\circ = -266.977 + 2.440\times10^{-3}T - 0.209\times10^{-6}T^2 - 630.000T^{-1}$

$\Delta Gf^\circ = -266.977 - 2.440\times10^{-3}T\ln T + 0.209\times10^{-6}T^2 - 315.000T^{-1} + 64.382\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (238). Low-temperature heat capacities from Kelley (118). High-temperature data based on Coughlin (42) and Chekhovskoi (35).

$ZrO_2(g)$

Zirconium Dioxide (ideal gas)

[Formation: $Zr(c,1) + O_2(g) = ZrO_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.009	65.402	65.402	0	-68.400	-70.510	51.685
300	11.026	65.470	65.403	.020	-68.404	-70.523	51.375
400	11.818	68.756	65.843	1.165	-68.609	-71.197	38.900
500	12.378	71.457	66.705	2.376	-68.796	-71.822	31.393
600	12.759	73.750	67.693	3.634	-68.985	-72.410	26.375
700	13.022	75.738	68.704	4.924	-69.186	-72.965	22.781
800	13.207	77.489	69.694	6.236	-69.407	-73.492	20.077
900	13.342	79.053	70.649	7.564	-69.647	-73.987	17.966
1000	13.442	80.464	71.561	8.903	-69.910	-74.456	16.272
1100	13.519	81.749	72.430	10.251	-70.195	-74.896	14.880
1136	13.540	82.185	72.732	10.738	-70.303	-75.049	14.438
1136	13.540	82.185	72.732	10.738	-71.254	-75.049	14.438
1200	13.578	82.928	73.256	11.606	-71.361	-75.259	13.706
1300	13.625	84.017	74.042	12.967	-71.543	-75.577	12.705
1400	13.663	85.028	74.792	14.331	-71.745	-75.879	11.845
1500	13.694	85.972	75.506	15.699	-71.966	-76.168	11.097
1600	13.720	86.856	76.187	17.070	-72.207	-76.439	10.441
1700	13.741	87.689	76.840	18.443	-72.467	-76.697	9.860
1800	13.759	88.475	77.465	19.818	-72.747	-76.937	9.341
1900	13.774	89.219	78.064	21.195	-73.047	-77.162	8.876
2000	13.787	89.926	78.640	22.573	-73.367	-77.371	8.455
2100	13.798	90.599	79.193	23.952	-73.708	-77.561	8.072
2125	13.800	90.762	79.328	24.297	-73.796	-77.608	7.982
2125	13.800	90.762	79.328	24.297	-78.796	-77.608	7.982
2200	13.808	91.241	79.726	25.332	-79.044	-77.563	7.705
2300	13.817	91.855	80.240	26.714	-79.378	-77.487	7.363
2400	13.824	92.443	80.736	28.096	-79.717	-77.396	7.048
2500	13.831	93.008	81.217	29.478	-80.061	-77.296	6.757
2600	13.837	93.550	81.680	30.862	-80.408	-77.176	6.487
2700	13.842	94.073	82.130	32.246	-80.760	-77.047	6.236
2800	13.847	94.576	82.565	33.630	-81.117	-76.900	6.002
2900	13.851	95.062	82.988	35.015	-81.478	-76.742	5.783
3000	13.855	95.532	83.398	36.401	-81.843	-76.575	5.578

Phase changes: 1136 K, α - β transition point of Zr; $\Delta H° = 0.951$ kcal/mol.
2125 K, melting point of Zr; $\Delta H° = 5.000$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 12.994 + 0.462\times10^{-3}T - 1.887\times10^{5}T^{-2}$

$H°- H°_{298} = 12.994\times10^{-3}T + 0.231\times10^{-6}T^{2} + 1.887\times10^{2}T^{-1} - 4.528$

$ZrO_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf° = -68.595 - 0.229\times10^{-3}T - 1.214\times10^{-6}T^2 + 110.600T^{-1}$

$\Delta Gf° = -68.595 + 0.229\times10^{-3}T\ln T + 1.214\times10^{-6}T^2 + 55.300T^{-1} - 8.713\times10^{-3}T$

1136-2000 K: $\Delta Hf° = -71.091 + 0.940\times10^{-3}T - 1.083\times10^{-6}T^2 + 165.100T^{-1}$

$\Delta Gf° = -71.091 - 0.940\times10^{-3}T\ln T + 1.083\times10^{-6}T^2 + 82.550T^{-1} + 1.837\times10^{-3}T$

2000-2125 K: $\Delta Hf° = -69.754 - 0.170\times10^{-3}T - 0.789\times10^{-6}T^2 - 419.700T^{-1}$

$\Delta Gf° = -69.754 + 0.170\times10^{-3}T\ln T + 0.789\times10^{-6}T^2 - 209.850T^{-1} - 6.608\times10^{-3}T$

2125-3000 K: $\Delta Hf° = -71.657 - 3.346\times10^{-3}T + 0.022\times10^{-6}T^2 - 441.300T^{-1}$

$\Delta Gf° = -71.657 + 3.346\times10^{-3}T\ln T - 0.022\times10^{-6}T^2 - 220.650T^{-1} - 28.319\times10^{-3}T$

Source: Data from JANAF (51).

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