

Six Methods for Estimating the Formation Enthalpy of Organic Compounds

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ABSTRACT

Finding published enthalpy of formation values for organic compounds is not always possible. Six methods are outlined for estimating this property, each utilizing different data that is generally readily available in one form or another. Additionally, a dozen different references for published thermodynamic data are provided.

Keywords: enthalpy of formation, heat of combustion, higher heating value, HHV, Benson group, flame temperature, free energy minimization

Introduction

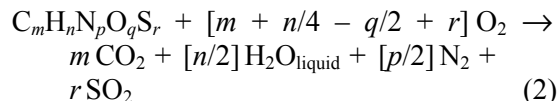
The *enthalpy of formation* ($\Delta_f H^\circ$) represents the energy required to form a molecule from its constituent elements in their standard states.^[1] It is required as part of the input data set for *free energy minimization* programs such as *PEP*^[2,3] or *CEA400*.^[4] Tabulated values may be found for various organic and inorganic compounds in a number of handbooks. The required value for a pure compound or complex mixture is sometimes not available. The different methods outlined in this article demonstrate ways of estimating the required value from information that is generally readily available, though sometimes from disparate or seemingly unrelated sources. All thermodynamic quantities are at standard conditions of 298.15 K and 1 bar pressure. All estimates of the $\Delta_f H^\circ$ in the following examples are for the solid phase.

Heat of Combustion

The *heat of combustion* ($\Delta_c H^\circ$) of a substance represents the heat evolved when that substance is completely converted to standard oxidation products by reaction with molecular oxygen.^[5] Equation 1 equates the $\Delta_c H^\circ$ to the sum of the $\Delta_f H^\circ$ of the products minus the sum of the $\Delta_f H^\circ$ of the reactants.^[1]

$$\Delta_c H^\circ = \sum \Delta_f H^\circ \text{ products} - \sum \Delta_f H^\circ \text{ reactants} \quad (1)$$

Equation 2 represents the ideal combustion of an organic compound composed of the elements C, H, N, O, and S:



The standard $\Delta_f H^\circ$ of the products, in kJ/mole, are found in Table 1.

Table 1. Standard Heats of Formation of Combustion Products at 298.15 K and 1 Bar.^[6]

Combustion Product	$\Delta_f H^\circ$ (kJ/mole)
CO ₂	-393.522
H ₂ O _(liquid)	-285.830
H ₂ O _(gas)	-241.826
O ₂	0.0
N ₂	0.0
SO ₂	-296.842

Tabulated values of the $\Delta_c H^\circ$ are sometimes found where the $\Delta_f H^\circ$ is not. To convert from

Example 1: The combustion enthalpy of *stearic acid*, $C_{18}H_{36}O_2$ (57-11-4), is -11280.4 kJ/mol.^[7]

$C_{18}H_{36}O_2$, $m = 18$, $n = 36$, $p = 0$ (no nitrogen present), $q = 2$, $r = 0$ (no sulfur present)

$\Delta_c H$	=	$\Sigma \Delta_f H^\circ$ (products)	-	$\Sigma \Delta_f H^\circ$ (reactants)
-11280.4	=	$m \Delta_f H^\circ CO_2 + [n/2] \Delta_f H^\circ H_2O_{liquid}$	-	$\Delta_f H^\circ C_{18}H_{36}O_2 + [m + n/4 - q/2 + r] \Delta_f H^\circ O_2$
-11280.4	=	$18 \Delta_f H^\circ CO_2 + [36/2] \Delta_f H^\circ H_2O_{liquid}$	-	$\Delta_f H^\circ C_{18}H_{36}O_2 + [18 + 36/4 - 2/2] \Delta_f H^\circ O_2$
-11280.4	=	$18 \Delta_f H^\circ CO_2 + 18 \Delta_f H^\circ H_2O_{liquid}$	-	$\Delta_f H^\circ C_{18}H_{36}O_2 + 26 \Delta_f H^\circ O_2$
-11280.4	=	$18 (-393.522) + 18 (-285.830)$	-	$\Delta_f H^\circ C_{18}H_{36}O_2 + 26(0.0)$
-11280.4	=	$-7083.40 + -5144.94$	-	$\Delta_f H^\circ C_{18}H_{36}O_2$

$C_{18}H_{36}O_2$, -947.94 kJ/mole

This compares favorably to a reference value^[7] of -947.7 kJ/mol.

one to the other, simply solve for the unknown in equation 1 using equation 2. See Example 1.

Note: because O_2 and N_2 are already *elements in their standard states*, their reference $\Delta_f H^\circ$ is 0.0 and thus can be ignored* in these computations. Generally, other elements present in many reactants, such as chlorine, are in trace quantities and do not influence the estimate significantly. If a reactant is considered that does include additional elements in non-trivial quantities, they would be handled in the same manner as described in example 1 for the CHONS system.

Higher Heating Value

Higher heating value, sometimes abbreviated *HHV*, or referred to as *caloric value*^[8] or *calorific value*,^[9] is actually the enthalpy of combustion in disguise; the sign is merely reversed by convention. It is usually used for complex or poorly characterized fuels such as coal and wood. The calculations made are the same as those described in example 1 for the $\Delta_c H^\circ$. The *lower heating value* is calculated in the same fashion as the higher heating value except that H_2O is in a *gaseous* rather than *liquid* form. It is usually preferable to convert the data from mass-based to formula-based so that the calculation of the product coefficients is simplified, and because many free energy minimization programs use formula-based data as input. This conversion requires the atomic weights of the elements involved. See example 2.

An equation^[10] that is sometimes used in estimating the HHV of biomass materials is:

$$HHV \text{ in MJ/Kg} = 0.63 + 0.39C \quad (3)$$

where C is the whole-number percentage of carbon. This equation was fit to 74 different fuels, and resulted in an r^2 (quality of fit) value of 0.894. It is valid for many biomass fuels that have low concentrations of waxes and oils. The effective range of carbon for this equation is between 33 and 55 percent.

* An additional correction may be made to account for the *change* in moles of *gaseous* species if the heat flow measurement were made in a constant-volume device such as a bomb calorimeter. It is not covered in this article due to this contribution typically only accounting for a correction of less than 0.5%.^[11]

Example 2: A charcoal manufactured from sawdust and pine bark, pyrolyzed at 400 °C, was shown to have a HHV of 12094 BTU/lb and an ultimate analysis of^[11] C 75.3%, H 3.8%, O 15.2%, N 0.8%, S 0.0%, and Ash 3.4%.

First, convert from BTU/lb to kJ/kg and HHV to $\Delta_c H$ (reverse sign):

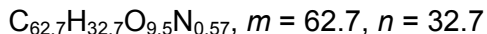
$$-28131 \text{ kJ/kg} = 12094 \text{ BTU/lb} \times 2.326 \times -1$$

Next, convert percent mass to moles per kilogram:

Element	% mass	g	Atomic ^[7] Weight (g/mol)	mol/kg
C	75.3	753	12.011	62.7
H	3.8	38	1.00794	37.7
O	15.2	152	15.9994	9.50
N	0.8	8	14.00674	0.57
S	0.0	0	32.066	0
Ash	3.4	34	NA	NA

Because the original form and composition of the elements that comprise the ash portion are unknown, it is assumed that it makes no significant contribution to the $\Delta_f H^\circ$. The resulting formula is $C_{62.7}H_{32.7}O_{9.5}N_{0.57}$. Since the molecular weight of this compound is 1 kg/mole, the $\Delta_c H$ of -28131 kJ/kg is also -28131 kJ/mole .

Using equations 1 and 2, solve for the reactant $\Delta_f H^\circ$:



$\Delta_c H$	=	$\Sigma \Delta_f H^\circ$ (products)	-	$\Sigma \Delta_f H^\circ$ (reactants)
-28131	=	$62.7 \Delta_f H^\circ \text{ CO}_2 + [32.7/2] \Delta_f H^\circ \text{ H}_2\text{O}_{\text{liquid}}$	-	$\Delta_f H^\circ C_{62.7}H_{32.7}O_{9.5}N_{0.57}$
-28131	=	$62.7(-393.522) + 16.35(-285.830)$	-	$\Delta_f H^\circ C_{62.7}H_{32.7}O_{9.5}N_{0.57}$
-28131	=	$-24674 + -4673$	-	$\Delta_f H^\circ C_{62.7}H_{32.7}O_{9.5}N_{0.57}$

$\Delta_f H^\circ$ for $C_{62.7}H_{32.7}O_{9.5}N_{0.57}$ is -1216 kJ/mol .

Benson Group Additivity

When the exact chemical structure of the compound is known, and it is composed of any of the elements *CHONS* or *halogens*, then a simple algorithm may be used to estimate the $\Delta_f H^\circ$ of the compound: the *Benson Group Additivity* method. Most “fragmentation” methods are limited to gas phase estimates. The method of Benson is an exception. It was extended to the liquid and solid phases by Domalski and Hearing,^[12] and is available in a software implementation.^[13] This method also estimates the heat capacity, entropy, entropy of formation,

Gibbs energy of formation, and the natural logarithm of the equilibrium constant for the formation reaction.^[12,13] This database was created from the analysis of 1512 different organic compounds.^[13]

First, the molecule is “broken down” into groups. A group generally defines the unique combination of the non-hydrogen atom of interest and the atoms that are immediately bonded to it. A few of the groups, such as the carboxyl that is present in carboxylic acids, are composed of two non-hydrogen atoms (carbon and oxygen in this case) instead of one. Next, after these groups have been identified, additional

correction groups are identified where applicable. These corrections account for such things as next-to-nearest-neighbor ring substitution interactions, ring strain corrections, etc. Lastly, the thermodynamic values assigned to each of

the selected groups are added, and the sum is the estimation of the properties for the molecule. The results are surprisingly accurate despite the simplicity of the method.

Example 3: Estimate the $\Delta_f H^\circ$ of cinnamic acid
 $C_9H_8O_2$ (621-82-9).

In Figure 1, each group has been numbered to facilitate their identification. What is not shown, which is typical of molecular renderings, are the hydrogen atoms bonded to the carbon atoms. This method uses its own, simple nomenclature to describe the component groups. Figure 1 shows that atoms 2 through 6 are fundamentally the same: a benzene ring carbon bonded to two benzene ring carbons and a hydrogen atom (that is not shown). In Benson notation, this is $C_B-(C_B)_2(H)$. Table 2 lists the component groups, including the $\Delta_f H^\circ$ values from reference 13.

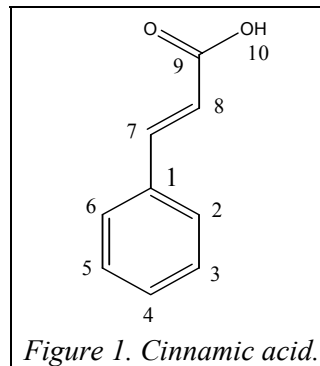


Table 2. Benson Groups and $\Delta_f H^\circ$ Values^[13] for Cinnamic Acid.

Group	Group Code	Qty.	Group $\Delta_f H^\circ$ (kJ/mol)	Total $\Delta_f H^\circ$ (kJ/mol)
1	$C_B-(C_B)_2(C_D)$	1	20.27	20.27
2-6	$C_B-(C_B)_2(H)$	5	6.53	32.65
7	$C_D-(C_B)(H)$	1	17.53	17.53
8	$C_D-(CO)(H)$	1	7.82	7.82
9	$CO-(C_D)(O)$	1	-134.10	-134.10
10	$O-(H)(CO)$	1	-282.15	-282.15
Total:				-337.98

This compares extremely well to a reference^[14] value of -337.23 kJ/mol.

Partial Benson Groups

Sometimes it is not convenient to “build from scratch” an entire molecule using Benson Groups. This may be due to the number of groups required to model the molecule, or, more likely, data for a required group does not exist and would render the estimate incomplete. It is certainly possible to create new groups—see reference 15 for how isocyanate groups were

evaluated. For “one-shot” estimates this may be more work than is necessary. A shortcut is to use what the author coined as a *Partial Benson Group* approach. This method relies on having the $\Delta_f H^\circ$ value for a molecule that is very similar in structure to the molecule with the unknown value. Subtracted from this “known” molecule are the groups and their respective $\Delta_f H^\circ$ values that do not belong, and then the ones required for the “unknown” molecule are added in yielding the estimate. See example 4.

Example 4: Estimate the $\Delta_f H^\circ$ of *cinnamic acid*, $C_9H_8O_2$ (621-82-9) using Partial Benson Groups. See Figure 1.

p-coumaric acid (Figure 2), $C_9H_8O_3$ (7400-08-0) $\Delta_f H^\circ$ -529.69 kJ/mol,^[16] is very similar in structure to cinnamic acid (see Figure 1). The only difference is the hydroxyl group at the “bottom” of the benzene ring. The group that is needed is $C_B-(C_B)_2(H)$, but instead there are two groups at that location: $C_B-(C_B)_2(O)$ and $O-(C_B)(H)$. By subtracting the two that are not needed, and adding the one required, the Partial Benson Group estimate is made. See Table 3.

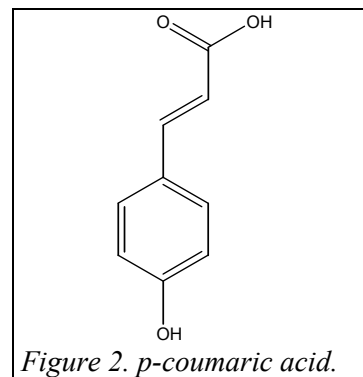


Table 3. Partial Benson Groups Estimation Method: Groups and $\Delta_f H^\circ$ Values.^[13]

Add/Subtract	Group Code	Qty.	Group $\Delta_f H^\circ$ (kJ/mol)	Total $\Delta_f H^\circ$ (kJ/mol)
<i>p</i> -coumaric acid $\Delta_f H^\circ$:		1	NA	-529.69
Add	$C_B-(C_B)_2(H)$	1	6.53	6.53
Subtract	$C_B-(C_B)_2(O)$	-1	1.00	-1.00
Subtract	$O-(C_B)(H)$	-1	-199.25	199.25
Total				-324.91

This compares favorably to a reference^[14] value of -337.23 kJ/mol.

Flame Temperatures

If the chemical formula of a compound is known (or calculated from an elemental analysis), but the structure is unknown, then using Benson Groups is ruled out. However, if a known pyrotechnic formulation using the compound has a measured flame temperature, then the $\Delta_f H^\circ$ may be “reverse-engineered” using a free energy minimization code. This assumes that

- The measured flame temperature is accurate.
- Chemical reactions proceed instantly (chemical kinetics are ignored).
- Combustion is complete at the temperature measurement location and does not include artifacts such as air entrainment cooling or afterburning that might alter the measured flame temperature and composition.
- The free energy minimization code can accurately model the product composition at the specified temperature and pressure, and includes all species that would realistically

be expected to be present in significant quantities.

- Gas/particle kinetic energy, condensed species velocity-lag, loss of energy by thermal radiation, etc. are all ignored.

In an ideal, adiabatic flame, where no heat is gained or lost, the enthalpy of the products equals that of the reactants.^[9] The free energy minimization code provides output of the combustion products present, their molar quantities, and the sum of their respective enthalpies at the stated conditions of temperature and pressure. Subtracting the sum of the $\Delta_f H^\circ$ of the reactants from the sum of the known $\Delta_f H^\circ$ of the products yields a useful (and optimistic) $\Delta_f H^\circ$ value for the unknown reactant. Due to the assumptions outlined above, this $\Delta_f H^\circ$ may be better regarded as a practical value than as an absolute one. See example 5.

Example 5: Estimate of $\Delta_f H^\circ$ based on flame temperature.

Shimizu^[17] has measured the flame temperatures of many colored flames. *Shellac* (9000-59-3) was used as the fuel/binder. Its formula is $C_6H_{9.6}O_{1.6}$.^[17] Estimate the $\Delta_f H^\circ$ based on the following formulation at a measured temperature of approximately 2475 K.^[17]

Ingredient	Formula	Percent	$\Delta_f H^\circ$ (kJ/mol)
Ammonium perchlorate	NH_4ClO_4	71	-295.3 ^[7]
Shellac	$C_6H_{9.6}O_{1.6}$	14	NA
Strontium carbonate	$SrCO_3$	10	-1220.1 ^[17]
Sodium oxalate	$Na_2C_2O_4$	5	-1317.96 ^[18]

Reviewing the results of the author's free energy minimization code,^[19] see Table 4, the difference in enthalpy between the products and the reactants is -52.30 kJ for 0.1304 moles of shellac. Thus, for this particular run, the $\Delta_f H^\circ$ per mole of shellac is $-52.30 \div 0.1304$, or -401.07 kJ/mole. This same procedure was used to evaluate 15 other data sets, and the overall "reverse-engineered" average was -440 kJ/mole. The tabulated results will appear in "Organic Fuels: Composition and Formation Enthalpy Part II: Resins, Charcoal, Pitch, Gilsonite, and Waxes".^[20]

Table 4. CEQ58 Specified Flame Temperature Run.

Propellant Composition:

Ingredient	Percent	moles	$\Delta_f H^\circ$ (kJ/mol)	Molecular Weight
Ammonium perchlorate	71.00%	0.6043	-295.3000	117.4888
Shellac	14.00%	0.1304	0.0000	107.3413
Strontium carbonate	10.00%	0.0677	-1220.1000	147.6292
Sodium oxalate	5.00%	0.0373	-1317.9600	133.9991

Enthalpy of Reactants ($\Delta_f H^\circ$) = -310.278 kJ/100 g

Element	Mole Fractions
C	11.1092
O	47.6526
H	3.6985
N	8.4645
Cl	21.4245
Na	1.7157
Sr	5.9351

Convergence Tolerance = 1×10^{-6}

Table 4. CEQ58 Specified Flame Temperature Run (continued).

Species with mole fractions ≥ 0.00001 :

Product	Species	Mole %	Mass
Water	H ₂ O	0.42226	26.24791
Carbon Dioxide	CO ₂	0.15795	23.98440
Carbon Monoxide	CO	0.11011	10.64219
Hydrogen Chloride	HCl	0.10763	13.54075
Nitrogen	N ₂	0.08719	8.42716
Hydrogen	H ₂	0.04850	0.33735
Sodium Chloride	NaCl	0.02073	4.17942
Strontium Chloride	SrCl ₂	0.01946	10.64207
Hydroxyl	OH	0.00887	0.52065
Chlorine	Cl	0.00777	0.95088
Hydrogen	H	0.00496	0.01726
Oxygen	O ₂	0.00212	0.23392
Nitrogen Oxide	NO	0.00077	0.07987
Sodium	Na	0.00063	0.04979
Oxygen	O	0.00059	0.03251
Sodium Hydroxide	NaOH	0.00027	0.03727
Strontium Chloride	SrCl	0.00008	0.03348
Strontium Hydroxide	Sr(OH) ₂	0.00008	0.03461
Strontium Hydroxide	SrOH	0.00001	0.00453

Mass fractions: Gas = 100.000 Condensed = 0.000

$\Delta_f H^\circ$ Reactants	=	-310.278	Temperature	=	2475 K
$\Delta_f H^\circ$ Gas	=	-362.583	$\Delta_f H^\circ$	=	-52.3049
Total Mass	=	100 g	Gas Molecular Weight	=	28.982
$\Delta_f H^\circ$ All	=	-362.583	Pressure	=	1.0 Bar
$\Delta_f H^\circ$ Condensed	=	0			

General Equations

If all else fails, and the *only* information available is the formula or composition of the reactant of interest, and it is composed of a subset of the elements CHO and N, then a “one size fits all” approach may be used. The author fitted a 2-dimensional equation for compounds containing only C and H, and 3-dimensional equations for compounds containing CHO, CHN, and CHON, to 1029 published $\Delta_f H^\circ$ (kJ/kg) values.^[14] The resulting equations may be used

to estimate *tentative* $\Delta_f H^\circ$ values if this is the *only* option available. While the CHO equation provides reasonably accurate values, the quality of the fit (r^2 parameter) for the other equations is not as good. Care must be exercised to stay within the boundaries of the input parameters; the equations used are polynomials, which are not well-behaved outside of the ranges specified. Don't divide by zero in equation 6 either! The results of the curve-fits are summarized in Table 5, the equations follow, and their respective parameters are listed in Table 6.

Table 5. Generic Equations, Percent Mass Basis Ranges, and Properties for $\Delta_f H^\circ$ Estimation of CHON Compounds.

Elements	Data Points	Ranges (min above, max below)				r^2	equation
		% C	% H	% O	% N		
CH	141	84.12	4.79			0.713	4
		95.21	15.88				
CHO	337	25.54	1.77	3.99		0.941	5
		89.34	14.14	71.08			
CHN	121	14.12	0.00		4.87	0.701	6
		88.28	12.08		83.31		
CHON	430	7.95	0.00	4.70	5.20	0.672	7
		81.63	13.02	63.99	74.44		

Equations:

$$y = a + bx^2 + cx^4 + dx^6 + ex^8 + fx^{10} \quad (4)$$

$$z = a + bx + cx^2 + dx^3 + ex^4 + fx^5 + gy + hy^2 + iy^3 + jy^4 + ky^5 \quad (5)$$

$$z = a + b/x + c/x^2 + d/x^3 + e/x^4 + f/x^5 + gy + hy^2 + iy^3 + jy^4 + ky^5 \quad (6)$$

$$z = a + bx + cy + dx^2 + ey^2 + fxy + gx^3 + hy^3 + ixy^2 + jx^2y \quad (7)$$

Table 6. Coefficients for Equations 4 through 7.

Coefficient	Equation			
	4	5	6	7
a	-2.5167e+07	3917.458641	21587.57325	-14380.3534
b	15831.82837	-634.043083	-1.9311e+06	5609.81255
c	-3.97590273	-26.7411923	-4.1661e+07	800.7687216
d	0.000498100	1.271410128	3.68535e+09	-670.056188
e	-3.1124e-08	-0.01593669	-7.0368e+10	-13.7322841
f	7.75955e-13	6.58264e-05	4.1961e+11	-197.843919
g		234.1069658	417.5059918	24.58584338
h		-5.30220462	-15.8927766	0.080091831
i		0.236528783	0.785609498	1.364527331
j		-0.00345384	-0.01411732	9.700068352
k		1.05262e-05	8.5484e-05	
x	% C	% C	% C	% O
y	$\Delta_f H^\circ$	% O	% N	% H
z	—	$\Delta_f H^\circ$	$\Delta_f H^\circ$	$\Delta_f H^\circ$

Curiously, equation 7 had the best r^2 value when O and H were used as opposed to any other combination or ratio of C, H, O, and N.

Conclusion

As illustrated, if a published $\Delta_f H^\circ$ value is not readily available, a value may be estimated using a variety of different methods. In addition to the cited references for published $\Delta_f H^\circ$ data, the reader may find the following titles of value:

- *Selected Values of Chemical Thermodynamic Properties, Part I. Tables, Circular 500*, F. D. Rossini, D. D. Wagman, W. H. Evans, S. Levine, and J. Jaffe, United States Department of Commerce, 1952.
- *Thermodynamic Constants of Inorganic and Organic Compounds*, M. Kh. Karapet'yants and M. L. Karapet'yants (translated from Russian by J. Schmorak), Ann Arbor Humphrey Science Publishers, 1970.
- *Sussex-N.P.L. Computer Analysed Thermochemical Data: Organic and Organometallic Compounds*, J.B. Pedley and J. Rylance, Sussex University, 1977.
- *Thermodynamic Data for Mineral Technology*, L. B. Pankratz, J. M. Stuve, and N. A. Gokcen, *Bureau of Mines Bulletin 677*, United States Department of the Interior, 1984.
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- 13) *THERM, NIST Estimation of the Chemical Thermodynamic Properties of Organic Compounds at 298.15 K* computer program Version 5.2, NIST Standard Reference Database 18, U.S. Department of Commerce, 1994. [See Reference 12.]
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