Selected Values of Heats of Combustion and Heats of Formation of Organic Compounds Containing the Elements C, H, N, O, P, and S*

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Selected values of the heats of combustion and heats of formation of 719 organic compounds are reported here. The data tabulated pertain to compounds containing the elements carbon, hydrogen, nitrogen, oxygen, phosphorus, and sulfur (CHNOPS). The information is arranged according to classes of compounds and within each class, compounds are arranged by empirical formula. The general classes covered are: hydrocarbons, alcohols, phenols, polyols, ethers, aldehydes, ketones, acids, acid anhydrides, esters, steroids, lactones, carbohydrates, heterocyclic oxygen compounds, amines, amides, urea derivatives, guanidine derivatives, amino acids, peptides, alkaloids, heterocyclic nitrogen compounds, porphyrins, organic sulfur compounds, and organic phosphorus compounds. When a selection was made from among several investigators, commentary is provided to indicate the choice, and usually some relevant data. The number of references cited is 596. An alphabetical compound index is provided which gives the name, page number, empirical formula, and the Wiswesser Line Notation (WLN), for each compound.

Key words: CHNOPS compounds; heat of combustion; heat of formation; selected values.

Contents

1. Introduction

As part of a continuing program of collecting and evaluating data on the thermodynamic properties of organic compounds, selected values are reported here for the heats of combustion and heats of formation of 719 organic compounds containing the elements carbon, hydrogen, nitrogen, oxygen, phosphorus, and sulfur (CHNOPS). Certain classes of compounds, such as amino acids, carbohydrates, glyceryl esters, and peptides, have been covered exhaustively because of their prime relevance to biological processes. Other classes of compounds, such as hydrocarbons, alcohols, acids, ketones, esters, aldehydes, were treated in a more cursory and limited manner. These latter classes contain compounds of natural biological occurrence, and have been included because a large group of common organic substances, such as ethanol, acetic acid, acetone and the like, have structures and interactions equivalent or similar to substances occurring in biological systems. The latter classes are also needed to provide a sufficient amount of combustion data on organic structures so that estimates can be made for molecules having a related structure, but for which there are no experimental data.

Over the course of the CHNOPS program, the coverage of the kind and number of compounds for which combustion data have been examined has increased from about 60 to the present value of 719. The literature has been searched from as far back as the 1840's up to the early part of 1970. The number of organic compounds for which experimental heats of combustion have been determined has grown from about 600 prior to 1900, to about 1500 by 1930, and to about 4000 for a current value (1970). Compounds containing the ele-

ments C, H, N, O, P, and S comprise about 3200 of this current total. We have arbitrarily selected 719 substances which we felt were of prime interest in biology. Considerable care has been taken in the evaluation and selection processes to present as unified a set of data as possible so that meaningful comparisons can be made among the data. We feel that this information on the heats of combustion and heats of formation of the CHNOPS compounds will be of general use to biochemists, biophysicists, and biologists as they make thermodynamic assessments on various life processes.

It is virtually impossible to provide a concise summation of the general state of the combustion data in this manuscript because of the broad range of substances which is treated. Various comments can be found at the end of a given table assessing the data on that class of compounds as were deemed necessary, along with the individual commentary on specific compounds. Qualitatively speaking, the combustion data on the hydrocarbons, alcohols, ketones, n-aliphatic acids, ethers, methyl esters, and amines are very good. The data on the amino acids and organic sulfur compounds can be rated as good to fair; those on the heterocyclic nitrogen compounds as a whole are good; those on carbohydrates and glyceryl esters are fair to poor, while the data on the steroids, alkaloids, porphyrins and organic phosphorus compounds can be rated, in general, as poor. A semiquantitative method for rating the combustion data can be obtained by examining the number of decimal places to which a value is given. This is explained more fully in section 5.9.

2. Arrangement of the Data

The classes of compounds are arranged according to the general sequence: CH, CHO, CHN, CHNO, CHS, CHNOS, CHP, and CHOP, which denotes the elements they contain. Within each table for a class of compounds the empirical formula (column 1) governs the order in which compounds are listed. This is followed by the name and physical state (column 2) of the compound. The combustion data, $\Delta Hc°$, are expressed in kcal mol^{-1} (column 3), and correspond to one of the generalized combustion reactions below. The substances involved in the combustion process are present in their thermodynamic standard states; that is, the stable form of the substances at 25 °C and one atmosphere pressure. The formation data, $\Delta Hf°$, are expressed in kcal mol^{-1} (column 4), and were calculated by combining the appropriate data for the heats of formation of $CO_2(g)$, H_2O (liq), $H_3PO_4(c)$, and $H_2SO_4 \cdot 115H_2O$(liq) with the combustion data. The literature sources are given in the last column (column 5). When several references are cited for a compound, those references which were used to obtain the selected heat of combustion and formation are underlined. If only one reference is available, it is underlined. If two or more references are underlined, and no comments are provided for that compound at the end of the listing, one may assume that the data appearing in the underlined references are either identical, or stem from the same investigation

with only minor changes due to recalibration or recalculation by the cited authors. If two or more references are underlined and each represent different investigations, then a comment is made regarding that compound and how the references were used as the basis of the selected values. We have also provided an alphabetical compound index which gives the empirical formula, and Wiswesser Line Notation (WLN) for each compound, in addition to the page number where the combustion data appear.

All of the selected values of heats of combustion and formation are derived from experimental data except for L-serine, which is based upon an estimated value. A few of the compounds have their values based upon heats of reaction in solution, or have data on the heat of solution, fusion, vaporization, or sublimation combined with the combustion data. Discussion is provided for these compounds explaining what has been done. The combustion values cited by Kharasch [233] [1] were not used in any way. However, the references in his paper were a valuable means of obtaining the original combustion results so that the necessary corrections could be applied to them.

The selection process is based upon the personal and professional opinion of an evaluator after examining all
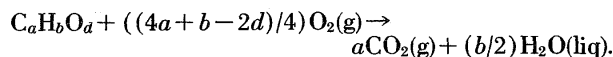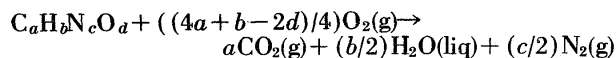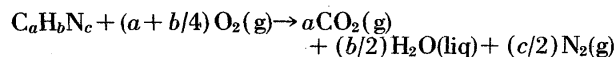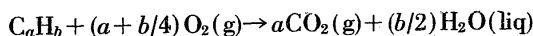
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[1] Figures in brackets indicate literature references (Section 7).

of the available data on a compound and after applying the appropriate corrections to the data. Factors which are often taken into consideration are: (1) sample purity, (2) number of experiments performed, (3) awareness of the investigators of the appropriate procedures, corrections, and constants, (4) agreement of the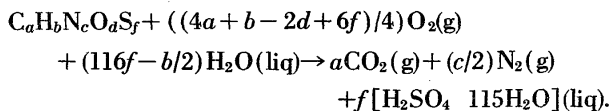 data with other investigation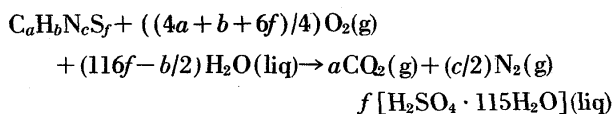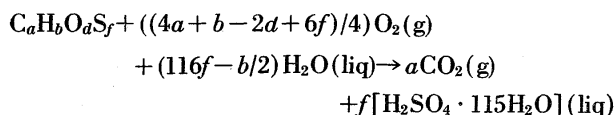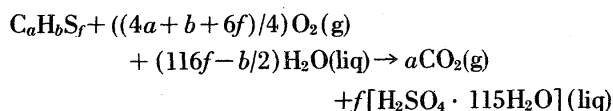s and (5) exposition of random and systematic errors. Cursory presentation of data, or lack of adequate discussion, often leaves persistent doubts as to the quality of the study. A well-documented presentation answers questions about the sample, the procedures, or the treatment of the results which most thermochemists would raise.

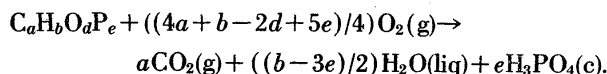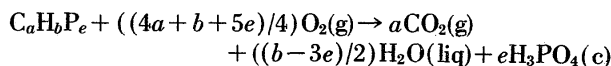## 3. Generalized Combustion Reactions for CHNOPS Compounds

In order to calculate the heats of formation of organic compounds of the type: C_aH_b, $C_aH_bN_c$, $C_aH_bN_cO_d$, or $C_aH_bO_d$ from their corresponding heats of combustion, only the heats of formation of $CO_2(g)$ and $H_2O(liq)$ are needed. Organic nitrogen compounds form $N_2(g)$ as a product in the combustion reaction which, by definition, has a heat of formation of zero.

$$C_aH_b + (a + b/4)O_2(g) \rightarrow aCO_2(g) + (b/2)H_2O(liq)$$

$$C_aH_bN_c + (a + b/4)O_2(g) \rightarrow aCO_2(g) \\ + (b/2)H_2O(liq) + (c/2)N_2(g)$$

$$C_aH_bN_cO_d + ((4a + b - 2d)/4)O_2(g) \rightarrow \\ aCO_2(g) + (b/2)H_2O(liq) + (c/2)N_2(g)$$

$$C_aH_bO_d + ((4a + b - 2d)/4)O_2(g) \rightarrow \\ aCO_2(g) + (b/2)H_2O(liq).$$

To calculate the heats of formation or organic compounds of the type: $C_aH_bS_f$, $C_aH_bO_dS_f$, $C_aH_bN_cS_f$, and $C_aH_bN_cO_dS_f$ from their corresponding heats of combustion, the heats of formation of $CO_2(g)$, $H_2O(liq)$ and $H_2SO_4 \cdot 115H_2O(liq)$ are needed. Care must be taken to account for the $((b/2) - f)H_2O(liq)$ formed as a product in these combustions, which is not written as a discrete product, but becomes incorporated into the aqueous sulfuric acid solution.

$$C_aH_bS_f + ((4a + b + 6f)/4)O_2(g) \\ + (116f - b/2)H_2O(liq) \rightarrow aCO_2(g) \\ + f[H_2SO_4 \cdot 115H_2O](liq)$$

$$C_aH_bO_dS_f + ((4a + b - 2d + 6f)/4)O_2(g) \\ + (116f - b/2)H_2O(liq) \rightarrow aCO_2(g) \\ + f[H_2SO_4 \cdot 115H_2O](liq)$$

$$C_aH_bN_cS_f + ((4a + b + 6f)/4)O_2(g) \\ + (116f - b/2)H_2O(liq) \rightarrow aCO_2(g) + (c/2)N_2(g) \\ f[H_2SO_4 \cdot 115H_2O](liq)$$

$$C_aH_bN_cO_dS_f + ((4a + b - 2d + 6f)/4)O_2(g) \\ + (116f - b/2)H_2O(liq) \rightarrow aCO_2(g) + (c/2)N_2(g) \\ + f[H_2SO_4 \; 115H_2O](liq).$$

To calculate the heats of formation of organic compounds of the type: $C_aH_bP_e$ and $C_aH_bO_dP_e$ from their corresponding heats of combustion, the heats of formation of $CO_2(g)$, $H_2O(liq)$, and $H_3PO_4(c)$ are required.

$$C_aH_bP_e + ((4a + b + 5e)/4)O_2(g) \rightarrow aCO_2(g) \\ + ((b - 3e)/2)H_2O(liq) + eH_3PO_4(c)$$

$$C_aH_bO_dP_e + ((4a + b - 2d + 5e)/4)O_2(g) \rightarrow \\ aCO_2(g) + ((b - 3e)/2)H_2O(liq) + eH_3PO_4(c).$$

4. Development of Combustion Calorimetry

The combustion studies of Andrews [10], and Favre and Silbermann [150], published around the middle of the 19th century, represent some of the very early work. Shortly thereafter, Thomsen began his classic combustion experiments using a flame calorimeter. His methods, and the results of his studies were published in a four volume compilation during the 1880's entitled "Thermochemishe Untersuchungen" [531]. Berthelot began his research in thermochemistry shortly after Thomsen. The advent of modern bomb calorimetry began with a publication by Berthelot and Vieille [73] in which they describe the combustion of substances in a bomb with oxygen under pressure.

Prior to 1900, the usual method of determining the energy (or water) equivalent was made by summing the products of the masses and specific heats of the various parts of the calorimeter. In 1903, Jaeger and von Steinwehr [203] reported the determination of the energy equivalent of their bomb calorimeter by means of electrical measurements. As a further improvement, they described the measurement of the temperature rise of their calorimeter using a platinum resistance thermometer [204] in conjunction with the electrical calibration. This brought the level of imprecision in their calibration experiments to about 2.5 parts in 10,000.

International agreement on a chemical standard to be used in calibrating bomb calorimeters came during the 1920's. The substance chosen was benzoic acid, and still today remains as the only chemical primary standard for this type of calibration. Improvements in calorimetric procedures, measuring instruments, and calculative methods reduced the inaccuracy of the energy of combustion of benzoic acid to 0.01 percent in the 1930's and led Washburn [559] to suggest the need for another refinement in bomb calorimetric calculations. The latter refinement deals with the reduction of combustion data from bomb conditions (certain mass of sample, pressure of oxygen, bomb volume and temperature) to conditions

in which both the reactants and products of the isothermal combustion reaction are at one atmosphere pressure. Subsequent development and improvement of the Washburn corrections were made by Hubbard, Scott, and Waddington (chapt. 5 in ref. [393]), and Prosen (chapt. 6 in ref. [393]). In 1949, the Commission on Thermochemistry of the International Union of Pure and Applied Chemistry began a project for the purpose of preparing a text which would place before the scientific community the best knowledge of the members and advisors of the Commission relative to experimental

thermochemistry and the measurement of heats of chemical reactions. The first volume of "Experimental Thermochemistry," edited by F. D. Rossini [393], was published in 1956. A second volume, edited by H. A. Skinner [437], was published in 1962.

Two valuable compilations were published during the course of gathering information for this manuscript; namely, the texts by Stull, Westrum, and Sinke [586], and Cox and Pilcher [587]. Both provide a vast amount of data on the thermochemistry and thermodynamics of organic compounds.

5. Corrections to the Combustion Data

From reading the preceding section on the development of combustion calorimetry, one can surmise that the experimental data have appeared in the literature in a variety of forms and with a variety of corrections. Sometimes the treatment of the data is presented clearly, sometimes not, and sometimes the reader is left to guess what the treatment is. We have attempted to bring all pertinent combustion data on organic compounds of interest to a common base by applying the appropriate corrections. This base is a reaction in which products and reactants are in their thermodynamic standard states at 298.15 K, with current values of the physical constants and units of measurement. An exception occurs with organic compounds containing sulfur in which the corresponding combustion product is $H_2SO_4 \cdot 115H_2O$ (liq). The latter is not a standard state, but a convenient final concentration.

For a pure liquid or crystal, the standard state is the substance in the condensed phase under a pressure of one atmosphere. For a gas, the standard state is the hypothetical ideal gas at unit fugacity, in which state the enthalpy is that of the real gas at the same temperature and at zero pressure. Symbolically, the standard state is designated by a superscript °.

The reference states for the elements C, H, N, O, P, and S are as follows:

For C, the reference state is crystalline graphite at 298.15 K and 1 atm pressure.
For H, N, and O, the reference state is the ideal diatomic gas at 298.15 K and unit fugacity. In this state, the respective enthalpy is that of the real gas at 298.15 K and zero pressure.
For P, the reference state is the crystalline white, α-modification at 298.15 K and 1 atm pressure.
For S, the reference state is the rhombic modification at 298.15 K and 1 atm pressure.

The heats of formation of the above elements in their reference states are defined as equal to zero.
The corrections, which have been applied to the experimental combustion data when necessary are as follows:

5.1. Calibration Correction

At the National Bureau of Standards, standard samples of benzoic acid are purified, the heat of combustion determined, and the combustion value certified [579] under the following conditions: (a) the combustion reaction is referred to 25 °C: (b) the sample is burned in a bomb of constant volume in pure oxygen at an initial pressure of 30 atm at 25 °C; (c) the number of grams of sample burned is equal to three times the

volume of the bomb in liters; (d) the number of grams of water placed in the bomb before combustion is equal to three times the volume of the bomb in liters.

No unnecessary departure should be made from the above certified conditions. The heat of combustion of the standard sample benzoic acid under conditions differing by small amounts from the standard conditions specified by (a), (b), (c), and (d) above will be obtained by multiplying the certified value by the factor, f, given below [579].

$$f = 1 + 10^{-6}[20(P - 30) + 42(m_s/V - 3) \\ + 30(m_w/V - 3) - 45(\theta - 25)]$$

where P is the initial pressure in atmospheres of oxygen at the temperature θ, to which the reaction is referred, m_s is the mass of the sample burned in grams, m_w is the mass of the water placed in the bomb in grams, and V is the internal volume of the bomb in liters.

If the value used by an investigator for the energy of combustion of benzoic acid differs significantly from the currently certified value, $-\Delta U_B = 26434 \pm 3$ Jg^{-1} (weighed in vacuum) [579], the combustion value under evaluation is multiplied by a ratio of the appropriate value to that used by the investigator.

5.2. Vacuum Correction

Particularly with the earlier literature, such as that of Stohmann or Berthelot, the combustion data presented were for the samples weighed in air. From estimates of the densities of the sample and of air (assuming a reasonable temperature, barometric pressure and relative humidity) a buoyancy correction is applied to reduce the weight of the sample to that in vacuum.

5.3. Molecular Weight Correction

The amount of the combustion reaction is often stated on the basis of the number of moles of substance burned, or of substance collected as a product. A significant correction may be required due to differences in the accepted values of atomic masses. Molecular weights are converted to the 1961 table of atomic masses based upon the isotope $C^{12} = 12$ [580].

5.4. Washburn Correction

This correction reduces bomb calorimetric data from bomb conditions to conditions in which the reactants and products are in their standard states at one atmospheric pressure.

5.5. ΔnRT Correction

The conversion of combustion data presented for the process at constant volume to that at constant pressure is made by means of the equation: $\Delta H^\circ = \Delta U^\circ + \Delta nRT$, where Δn is the difference between the number of moles of gaseous products and gaseous reactants involved in combustion reaction.

5.6. Temperature Correction

All combustion data are reduced to the reference temperature of 25 °C (298.15 K). The appropriate ΔCp for the combustion reaction is calculated or estimated for the temperature interval under consideration. The temperature 298 K is assigned to the ΔH_c° and ΔHf° data tabulated for the various classes of compounds in section 6, and is implied to be synonymous with 298.15 K.

5.7. Calculation of the Standard Heat of Formation

The standard heat of formation at 298.15 K of an organic compound is calculated from the standard heat of combustion and the heats of formation of carbon dioxide (g), -94.051 kcal mol^{-1}; water (liq), -68.315 kcal mol^{-1}; phosphoric acid (c), -305.7 kcal mol^{-1}; and aqueous sulfuric acid, $H_2SO_4 \cdot 115H_2O$, -212.192 kcal mol^{-1}. The latter heat-of-formation data were obtained from NBS Technical Note 270–3 [581].

5.8. Units and Constants

The evaluated heats of combustion and heats of formation are expressed in kcal mol^{-1}. The unit of energy in SI units is the joule, and one calorie is taken as 4.184 J. Values for the heats of combustion in kJ mol^{-1} can be obtained by multiplying the tabulated values in kcal mol^{-1} by 4.184. Calculation of the heats of formation in kJ mol^{-1} should be obtained from the difference between the heats of combustion and the corresponding sum of the heats of formation of the combustion products, both in kJ mol^{-1}. Following this path, rather than the multiplication of the tabulated heats of formation by 4.184, will avoid rounding variations in the last place which otherwise will occur.

The value of the gas constant, R, is 8.3143 J deg^{-1} mol^{-1}. The ice point is defined as 273.15 K.

5.9. Uncertainty of the Data

Although uncertainties are not cited, the number of significant figures used in reporting the combustion and formation data is related to the estimated uncertainty as shown below.

If ΔHc° or ΔHf° is cited to: (kcal mol^{-1})	The estimated uncertainty in ΔHc° or ΔHf° is: (kcal mol^{-1})
0.001	<0.05
0.01	0.05 to 0.5
0.1	0.5 to 2
1	2 to 20

5.10. Acknowledgements

6. Classes of Compounds and Selected Values

6.1. Aliphatic Hydrocarbons

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
CH_4	methane (g)	-212.79	-17.89	[10, 32, 150, 315, 387, 388, 530, 531, 578]
C_2H_2	acetylene (g)	-310.61	$+54.19$	[31, 32, 62, 315, 316, 531, 556, 578, 590,]
C_2H_4	ethylene (g)	-337.23	$+12.50$	[10, 32, 62, 141, 150, 168, 235, 315, 316, 375, 391, 531, 578]
C_2H_6	ethane (g)	-372.81	-20.24	[62, 390, 531, 578]
C_3H_8	propane (g)	-530.57	-24.84	[62, 390, 531, 578]
C_4H_{10}	n butane (g)	-687.68	-30.10	[390, 578, 589]
C_5H_{12}	n-pentane (g)	-845.16	-34.99	[359, 390, 578]
C_5H_{12}	n-pentane (liq)	-838.78	-41.37	[404, 373, 578, 584]
C_6H_{14}	n-hexane (liq)	-995.01	-47.50	[167, 209, 373, 466, 516, 576, 578]

The heats of combustion and formation of the selected values for the aliphatic hydrocarbons are consistent with those tabulated by Zwolinski et al. [578]. This tabulation (A.P.I. Project 44) has appeared in an earlier form which may be more familiar; see Rossini [392].

methane (g)—The combustion data of Rossini [387, 388] were used to make the selection. The early studies on the heat of combustion of methane by Andrews [10], Mixter [315], Favre and Silbermann [150], Thomsen [530,531] and Berthelot [32] are of historical interest only.

acetylene (g)—The unpublished calculated data of Prosen and Rossini cited by Wagman, Kilpatrick, Pitzer, and Rossini [556] were chosen for the selected value. The actual data source appears to be the hydrogenation studies of Conn, Kistiakowsky, and Smith [590], corrected to 25 °C. The early studies of Thomsen [531], Berthelot [31, 32], Berthelot and Matignon [62], and Mixter [315, 316] are of historical interest only.

ethylene (g)—The combustion data of Rossini and Knowlton [391], and the heat-of-hydrogenation data of Kistiakowsky, Romeyn, Ruhoff, Smith, and Vaughan [235] as corrected by Prosen and Rossini [375] were used to obtain the selected value. The early studies of Dulong [141], Grassi [168], Favre and Silbermann [150], Andrews [10], Berthelot [32], Berthelot and Matignon [62], Thomsen [531], and Mixter [315, 316] are of historical interest only.

ethane (g)—The combustion data of Rossini [390] were used to make the selection. The early studies by Thomsen [531], and Berthelot and Matignon [62] are of historical interest only.

propane (g)—The combustion data of Rossini [390] were used to make the selection. The early studies of Thomsen [531], and Berthelot and Matignon [62] are of historical interest only.

n-butane (g)—The combustion data of Rossini [390] and Prosen, Maron, and Rossini [589] were averaged to obtain the selected value.

n-pentane (g)—The combustion data of Rossini [390] were used to make the selection. The more recent data of Pilcher and Chadwick [359] are in very good agreement with the selection.

n-pentane (liq)—The combustion data of Prosen and Rossini [373] were used for the selected value. The recent data of Good [584] are in very good agreement with the selection. The earlier work of Roth and Macheleidt [404] was not used.

n-hexane (liq)—The combustion data of Prosen and Rossini [373] were used to make the selection. The data of Jessup [209] and Good and Smith [167] are in very good agreement with the selection. The early data of Stohmann and Kleber [466], and the data of Zubov [576] as corrected by Swietoslawski [516] are of historical interest only.

6.2. Alicyclic Hydrocarbons

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
C_3H_6	cyclopropane (g)	-499.85	$+12.75$	[32, 62, 63, 238, 578]
C_4H_8	cyclobutane (liq)	-650.22	$+0.76$	[113, 217, 578]
C_5H_{10}	cyclopentane (liq)	-786.55	-25.28	[113, 213, 448, 516, 577, 578]
C_6H_{12}	cyclohexane (liq)	-936.87	-37.33	[167, 213, 217, 317, 397, 448, 477, 478, 516, 576, 578]

6.2. Alicyclic Hydrocarbons—Continued

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
C$_7$H$_{14}$	cycloheptane (liq)	−1099.09	−37.47	[217, 448, 516, 576, 578]
C$_8$H$_{16}$	cyclooctane (liq)	−1258.35	−40.58	[217, 412, 419, 448, 578]

The selected values for the heats of combustion and formation of the alicyclic hydrocarbons are consistent with those tabulated by Zwolinski et al. [578]. This latter tabulation (A.P.I. Project 44) has appeared in an earlier form which may be more familiar; see Rossini [392].

cyclopropane (g)—The combustion data of Knowlton and Rossini [238] were chosen in preference to the earlier work by Berthelot [32], and Berthelot and Matignon [62, 63].

cyclobutane (liq)—The combustion data of Coops and Kaarsemaker [113] and Kaarsemaker and Coops [217] appear to be the same.

cyclopentane (liq)—The combustion data of Johnson, Prosen, and Rossini [213] were used in preference to the data of Kaarsemaker and Coops [217], and Spitzer and Huffman [448]. The work of Zubov [577] as corrected by Swietoslawski [516] is of historical interest only.

cyclohexane (liq)—The combustion data of Good and Smith [167] and Johnson, Prosen, and Rossini [213] were used to make the selection. The data of Kaarsemaker and Coops [217], Spitzer and Huffman [448], and Moore, Renquist and Parks [317] are in good agreement with the selection. The works of Stohmann and Langbein [477, 478], Zubov [576] as corrected by Swietoslawski [516], and of Roth and von Auwers [397] are of historical interest only.

cycloheptane (liq)—The combustion data of Spitzer and Huffman [448] and Kaarsemaker and Coops [217] were averaged to obtain the selected value. The data of Zubov [576] as corrected by Swietoslawski [516] were not used.

cyclooctane (liq)—The combustion data of Kaarsemaker and Coops [217], and Spitzer and Huffman [448] were averaged to obtain the selected value. The data of Schläpfer [419] and Ruzicka and Schläpfer [412] were not used.

6.3. Aromatic Hydrocarbons

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
C$_6$H$_6$	benzene (g)	−789.06	+19.81	[33, 64, 120, 151, 175, 184, 239, 285, 392, 483, 486, 531, 552, 567, 578]
C$_6$H$_6$	benzene (liq)	−780.96	+11.71	[31, 114, 115, 140, 167, 372, 379, 380, 381, 382, 383, 392, 397, 468, 483, 578]
C$_{10}$H$_8$	naphthalene (g)	−1249.4	+35.6	[4, 7, 83, 186, 311, 428, 430, 431, 507, 569, 573]
C$_{10}$H$_8$	naphthalene (c)	−1231.8	+18.0	[22, 26, 57, 69, 75, 86, 106, 138, 152, 197, 219, 225, 276, 313, 371, 377, 380, 385, 397, 410, 420, 447, 457, 458, 515, 522, 538, 544, 545, 546, 571]
C$_{14}$H$_{10}$	anthracene (g)	−1712.0	+53.7	[83, 186, 202, 231, 237, 329, 428, 455]
C$_{14}$H$_{10}$	anthracene (c)	−1687.3	+29.0	[22, 26, 74, 75, 86, 106, 158, 236, 276, 279, 313, 345, 377, 384, 429, 457, 468, 560]
C$_{14}$H$_{10}$	phenanthrene (g)	−1706.7	+48.4	[83, 186, 202]
C$_{14}$H$_{10}$	phenanthrene (c)	−1685.6	+27.3	[26, 74, 75, 106, 158, 236, 279, 313, 384, 429, 468]

6.3. Aromatic Hydrocarbons—Continued

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_{16}H_{10}$	pyrene (c)	−1873.83	+27.44	[384, 562]
$C_{16}H_{10}$	fluoranthene (c)	−1892.14	+45.75	[82, 562]
$C_{18}H_{12}$	triphenylene (c)	−2136.53	+33.72	[279, 562]
$C_{18}H_{12}$	chrysene (c)	−2137.8	+35.0	[279, 460]
$C_{18}H_{12}$	naphthacene (c)	−2141.1	+38.3	[279]
$C_{18}H_{12}$	1,2-benzanthracene (c)	−2144.0	+41.2	[279]
$C_{18}H_{12}$	3,4-benzphenanthrene (c)	−2147.3	+44.5	[279]
$C_{20}H_{12}$	perylene (c)	−2334.60	+43.69	[364, 562]

benzene (*g*)—References [120, 151, 175, 184, 239, 285, 392, 552, 567, 578] provided experimental data on the determination of the heat of vaporization of benzene. We have used the ideal heat of vaporization at 25 °C of 8.10 kcal mol^{-1} as in references [392, 578]. By combining the latter value with the $\Delta Hc°[C_6H_6(\text{liq})] = -780.96$ kcal mol^{-1}, we calculate $\Delta Hc° = -789.06$ kcal mol^{-1} for gaseous benzene. The early studies on the heat of combustion of gaseous benzene, references [33, 64, 483, 486, 531] were not used and are of historical interest only.

benzene (*liq*)—The combustion data of Good and Smith [167], and Prosen, Gilmont, and Rossini [372] were used to obtain the selected value. The data of Coops, Mulder, Dienske, and Smittenberg [114, 115] were not used. References [31, 140, 379–383, 397, 468, 483, 578] summarize the early studies, and are of historical interest only.

naphthalene (*g*)—The sublimation pressures of naphthalene were measured by Bradley and Cleasby [83], Sherwood and Bryant [430], Miller [311], Zil'berman-Granovskaya [573], Swan and Mack [507], Winstrom and Kulp [569], Allen [7], Hoyer and Peperle [186], Aihara [4], Sears and Hopke [428], and Shlyarenko, Markin, and Belyaeva [431]. When plotted individually as log P versus $1/T$, these sets of data show generally poor agreement, but when considered as a whole, good agreement results, giving a reasonably straight line. Using a least-squares treatment of the vapor pressure data, we obtain for the heat of sublimation, 17.6 kcal mol^{-1} at 25 °C. Combining this with our selection, $\Delta Hc°[C_{10}H_8(c)] = -1231.8$ kcal mol^{-1}, we calculate $\Delta Hc° = -1249.4$ kcal mol^{-1} for gaseous naphthalene.

naphthalene (*c*)—The heat of combustion of naphthalene (c) was measured by von Rechenberg [377], Stohmann [457, 458], Rübner [410], Richards and Davis [380], Berthelot and Louguinine [57], Berthelot and Recoura [69], Berthelot and Vieille [75], Fischer and Wrede [152], Riiber and Schetelig [385], Roth and von Auwers [397], Wrede [571], Dickinson [138], Karrar and Fioroni [219], Verkade and Coops [544, 545], Beckers [22], Burriel [86], Keffler [225], Milone and Rossignoli [313], Schläpfer and Fioroni [420], Huffman and Ellis [197], Bender and Farber [26], Speros and Rossini [447], Prosen and Colomina [371], Mackle and O'Hare [276], and Coleman and Pilcher [106]. The value for the heat of combustion of naphthalene relative to that of benzoic acid under bomb conditions was well-established by various experimenters as 1.5202 to 1.5204. For a discussion of this point see Verkade [538], Verkade, Coops and Hartman [546], Swietoslawski [515], and Swietoslawski and Starczewska [522]. If we take the value 1.5204, and the presently accepted value for benzoic acid $(-\Delta U_B = 26434\ \text{Jg}^{-1}$ (vacuum) at 25 °C), and apply the appropriate corrections (for standard states, ΔnRT, and calculation of $\Delta Hf°$), we obtain for our selected values $\Delta Hc° = -1231.8$ kcal mol^{-1}, and $\Delta Hf° = +18.0$ kcal mol^{-1}.

anthracene (*g*)—Sublimation pressures have been measured by Bradley and Cleasby [83], Stevens [455], Klochkov [237], Inokuchi, Shiba, Handa, and Akamatu [202], Sears and Hopke [428], Nitta, Seki, and Momotani [329], Kelly and Rice [231], and Hoyer and Peperle [186]. The experimental data of Bradley and Cleasby [83], and Klochkov [237] were used to obtain a selected heat of sublimation of 24.7 kcal mol^{-1}. By combining the latter with $\Delta Hc°[C_{14}H_{10}(c)] = -1687.3$ kcal mol^{-1}, we calculate $\Delta Hc° = -1712.0$ kcal mol^{-1} for gaseous anthracene.

anthracene (*c*)—The heat of combustion of anthracene (c) was measured by von Rechenberg [377], Stohmann [457], Stohmann, Kleber, and Langbein [468], Berthelot and Vieille [74, 75], Beckers [22], Burriel [86], Wiegert [560], Klaproth [236], Milone and Rossignoli [313], Fries, Walter, and Schilling [158], Shchukarev and Shchukareva [429], Richardson and Parks [384], Parks, West, Naylor, Fujii and McClaine [345], Bender and Farber [26], Magnus, Hartmann, and Becker [279], Mackle and O'Hare [276], and Coleman and Pilcher [106]. An average heat of combustion derived from the data of the last six investigations [26, 106, 276, 279, 345, 384], mentioned constitutes our selected value. $\Delta Hc°[C_{14}H_{10}(c)] = -1687.3$ kcal mol^{-1}.

phenanthrene (*g*)—Sublimation pressures were measured by Bradley and Cleasby [83], Inokuchi, Shiba, Handa, and Akamatu [202], and Hoyer and Peperle [186]. We derived the heat of sublimation at 25 °C of 21.1 kcal mol^{-1} from the data of Bradley and Cleasby [83]. By combining ΔH (sublimation) with $\Delta Hc°[C_{14}H_{10}(c)] = -1685.6$ kcal mol^{-1}, we calculate $\Delta Hc° = -1706.7$ kcal mol^{-1} for gaseous phenanthrene.

phenanthrene (*c*)—The heat of combustion of phenanthrene (c) was measured by Stohmann, Kleber, and Langbein [468], Berthelot and Vielle [74, 75], Klaproth [236], Milone and Rossignoli [313], Shchukarev and Shchukareva [429], Fries, Walter, and Schilling [158], Richardson and Parks [384], Bender and Farber [26], Magnus, Hartmann, and Becker [279], and Coleman and Pilcher [106]. An average heat of combustion derived from the data of the last three investigations [26, 106, 279], constitutes our selected value. $\Delta Hc°[C_{14}H_{10}(c)] = -1685.6$ kcal mol^{-1}.

pyrene (c)—The combustion data of Westrum and Wong [562] were preferred to those of Richardson and Parks [384] in making the selection.

fluoranthene (c)—The combustion data of Westrum and Wong [562], and Boyd, Christensen, and Pua [82] were averaged in obtaining the selected value.

triphenylene (c)—The combustion data of Westrum

and Wong [562] were preferred to those of Magnus, Hartmann, and Becker [279] in making the selection.
chrysene (c)—The combustion data of Magnus, Hartmann, and Becker [279] were preferred to those of Stohmann [460] in making the selection.
perylene (c)—The combustion data of Westrum and Wong [562] were preferred to those of Pongratz and Griengl [364] in making the selection.

6.4 Aliphatic Alcohols

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
CH$_4$O	methanol (g)	−182.72	−47.96	[150, 389, 531]
CH$_4$O	methanol (liq)	−173.64	−57.04	[92, 149, 151, 380, 395, 398, 406, 471, 555, 561]
C$_2$H$_6$O	ethanol (g)	−336.86	−56.19	[10, 150, 389, 531]
C$_2$H$_6$O	ethanol (liq)	−326.68	−66.37	[11, 12, 59, 60, 92, 101, 144, 151, 380, 406, 555]
C$_3$H$_8$O	1-propanol (liq)	−482.75	−72.66	[92, 261, 380, 445, 516, 575]
C$_3$H$_8$O	2-propanol (liq)	−479.44	−75.97	[92, 261, 342, 344, 445, 516, 575]
C$_4$H$_{10}$O	1-butanol (liq)	−639.53	−78.25	[92, 172, 320, 380, 438, 516, 532, 543, 575]
C$_4$H$_{10}$O	2-butanol (liq)	−635.90	−81.88	[92, 438]
C$_4$H$_{10}$O	2-methyl-1-propanol (liq)	−637.93	−79.85	[92, 261, 380, 438, 516, 575]
C$_4$H$_{10}$O	2-methyl-2-propanol (liq)	−631.92	−85.86	[438]
C$_4$H$_{10}$O	2-methyl-2-propanol (c)	−630.3	−87.5	[263, 376, 516, 575]
C$_5$H$_{12}$O	1-pentanol (liq)	−795.88	−84.27	[92, 171, 261, 516, 543, 575]
C$_6$H$_{14}$O	1-hexanol (liq)	−951.86	−90.65	[92, 543]

methanol (g)—The combustion data of Rossini [389] on gaseous methanol were chosen in preference to the early work of Thomsen [531]. A correction for dimer and tetramer formation amounting to −0.13 kcal mol^{-1} was made to the combustion data of Rossini [389] using the study of Weltner and Pitzer [561]. The data of Favre and Silbermann [150] are of historical interest only.
methanol (liq)—Our selected value for the heat of combustion of CH$_3$OH(liq) is obtained by combining the value for the heat of combustion of CH$_3$OH(g) with the heat of vaporization of the liquid to the gaseous monomer. The heat of vaporization of methanol at 25 °C was taken from the measurements of Fiock, Ginnings, and Holton [151], ΔHvap at 25 °C=8.95 kcal mol^{-1}. Recent vaporization data by Wadsö [555] are in very good agreement. By applying the dimerization data of Weltner and Pitzer [561] to the vaporization data, we obtain ΔHvap at 25°=9.08 kcal mol^{-1} for the process: CH$_3$OH(liq)=CH$_3$OH(g, monomer).

The recent combustion measurement of Chao and Rossini [92] on the liquid is in good agreement with our selection. The earlier works of Stohmann, Kleber, and Langbein [471], Richards and Davis [380], Roth

[395], Roth and Banse [398], Roth and Müller [406] and I. G. Farbenfabriken [149] have not been used.
ethanol (g)—The combustion data of Rossini [389] on gaseous ethanol were chosen in preference to the earlier data of Thomsen [531]. A correction for the presence of dimeric ethanol (g) was introduced into the combustion data from the data of Coburn and Grunwald [101] amounting to −0.06 kcal mol^{-1}. The data of Andrews [10] and Favre and Silbermann [150] are only of historical interest.
ethanol (liq)—Our selection for the heat of combustion was obtained by combining the value for the heat of combustion of CH$_3$CH$_2$OH(g) with the heat of vaporization of the liquid to the gaseous monomer. The heat of vaporization of ethanol at 25 °C was taken from the measurements of Fiock, Ginnings, and Holton [151], ΔHvap at 25 °C=10.13 kcal mol^{-1}. Recent vaporization data by Wadsö [555] are in very good agreement. By applying the dimerization data of Coburn and Grunwald [101] to the vaporization data, we obtain for the process: CH$_3$CH$_2$OH(liq)=CH$_3$CH$_2$OH (g, monomer), ΔHvap at 25 °C=10.18 kcal mol^{-1}.

The recent combustion measurement of Chao and Rossini [92] on the liquid are in good agreement with

our selection. The earlier data of Berthelot and Matignon [59, 60] Emery and Benedict [144], Atwater and Rosa [11], Atwater and Snell [12], Roth and Müller [406] and Richards and Davis [380] were not used.

1-propanol (liq) — The combustion data of Chao and Rossini [92] and Snelson and Skinner [445] were averaged to obtain the selected value. The earlier data were not used.

2-propanol (liq) — The combustion data of Chao and Rossini [92], Snelson and Skinner [445], and Parks, Mosley and Peterson [344] were averaged to obtain the selected value. The earlier data were not used.

1-butanol (liq) — The combustion data of Mosselman and Dekker [320], and Gundry, Head, and Lewis [172] were averaged to obtain the selected value. The early data of Zubov [575] and the correction of the latter by Swietoslawski [516] were not used. The combustion data of Tjebbes [532] appeared to be not negative enough by at least one kcal mol⁻¹, and hence were not used. The combustion data of Chao and Rossini [92] appeared too negative by about 0.4 kcal mol⁻¹.

The combustion data of Richards and Davis [380], Verkade and Coops [543], and Skinner and Snelson [438] were not used.

2-butanol (liq) — The combustion data of Chao and Rossini [92], and Skinner and Snelson [438] were averaged to obtain the selection.

2-methyl-1-propanol (liq) — The combustion data of Chao and Rossini [92] and Skinner and Snelson [438] were averaged to obtain the selected value. The earlier data were not used.

2-methyl-2-propanol (c) — The combustion data of Skinner and Snelson [438] on the liquid, and the heat-of-fusion data of Raley, et al. [376] were combined to obtain the selected value.

1-pentanol (liq) — The combustion data of Gundry, Harrop, Head, and Lewis [171] were used to obtain the selected value. The earlier data were not used.

1-hexanol (liq) — The combustion data of Chao and Rossini [92] were used to obtain the selected value, which agrees with the data of Verkade and Coops [543] by about 0.3 kcal mol⁻¹.

6.5. Phenols

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol⁻¹	$\Delta Hf°298$ K kcal mol⁻¹	Reference
C_6H_6O	phenol (c)	−729.80	−39.45	[9, 16, 57, 75, 118, 119, 218, 280, 341, 377, 457, 460, 476, 484]
$C_6H_6O_2$	pyrocatechol (c)	−683.0	−86.3	[457, 460, 476]
$C_6H_6O_2$	resorcinol (c)	−681.30	−87.95	[137, 457, 460]
$C_6H_6O_2$	hydroquinone (c)	−681.78	−87.47	[29, 57, 277, 280, 341, 363, 460, 476, 484, 523, 537]
C_7H_8O	o-cresol (c)	−882.72	−48.90	[9, 118, 119, 485]
C_7H_8O	m-cresol (c)	−885.25	−46.37	[9, 118, 119, 485, 510, 511]
C_7H_8O	p-cresol (c)	−883.99	−47.63	[9, 118, 119, 485]
$C_8H_{10}O$	2-ethylphenol (c)	−1044.07	−49.91	[77]
$C_8H_{10}O$	3-ethylphenol (c)	−1042.77	−51.21	[77]
$C_8H_{10}O$	4-ethylphenol (c)	−1040.35	−53.63	[77]

phenol (c) — The heat of combustion of phenol was measured by von Rechenberg [377], Stohmann [457, 460], Berthelot and Louguinine [57], Berthelot and Vieille [75], Andon, Biddiscombe, Cox, Handley, Harrop, Herington, and Martin [9], Cox [118, 119], Karlsson [218], Manchester [280], Parks, Manchester, and Vaughan [341], Stohmann, Rodatz, and Herzberg [484], Stohmann and Langbein [476], and Badoche [16]. We have used the data of Andon et al. [9] and Cox [118, 119] for our selected value.

pyrocatechol (c) — The combustion data of Stohmann [460], and Stohmann and Langbein [476] were obtained using an oxygen bomb calorimeter, and are preferred to the data of Stohmann [457] in which the potassium chlorate-oxidative mixture technique was used. The data in references [460] and [476] are the same. The heat of combustion calculated from the latter was found to be −684.9 kcal mol⁻¹ after all corrections were applied. This was adjusted to −683.0 kcal mol⁻¹ because the value for the heat of combustion of phenol found by Stohmann and Langbein [476] was 2 to 3

kcal mol⁻¹ more negative than our presently selected value for phenol.

resorcinol (c) — The combustion data of Desai, Wilhoit, and Zwolinski [137] were chosen in preference to the earlier combustion data.

hydroquinone (c) — The combustion data of Pilcher and Sutton [363] were chosen in preference to any other combustion data.

o-cresol (c) — The combustion data of Andon, Biddiscombe, Cox, Handley, Harrop, Herington, and Martin [9], and Cox [118, 119] were chosen in preference to the data of Stohmann, Rodatz, and Herzberg [485].

m-cresol (c) — The combustion data of Andon, Biddiscombe, Cox, Handley, Harrop, Herington, and Martin [9], and Cox [118, 119] were chosen in preference to the earlier data.

p-cresol (c) — The combustion data of Andon, Biddiscombe, Cox, Handley, Harrop, Herington, and Martin [9], and Cox [118, 119] were chosen in preference to the data of Stohmann, Rodatz and Herzberg [485].

6.6. Aliphatic Di- and Polyols

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_2H_6O_2$	1,2-ethanediol (liq) (ethylene glycol)	−284.35	−108.70	[216, 260, 322, 345, 476]
$C_3H_8O_2$	1,2-propanediol (liq)	−435.8	−119.6	[259, 322]
$C_3H_8O_2$	1,3-propanediol (liq)	−431.0	−124.4	[259]
$C_3H_8O_3$	1,2,3-propanetriol (liq) (glycerol)	−395.65	−159.76	[144, 260, 345, 457, 481]
$C_4H_{10}O_4$	meso-1,2,3,4-butanetetrol (c) (meso-erythritol)	−500.22	−217.56	[58, 270, 345, 457, 460, 476]
$C_5H_{12}O_4$	pentaerythritol (c)	−660.1	−220.0	[305, 476]
$C_5H_{12}O_5$	xylitol (c)	−612.83	−267.32	[330]
$C_5H_{12}O_5$	L-arabitol (c)	−611.4	−268.7	[476]
$C_6H_{12}O_3$	acetone glycerol (liq)	−811	−163	[17]
$C_6H_{14}O_6$	D-mannitol (c)	−722.97	−319.54	[17, 76, 162, 345, 377, 457, 476, 481]
$C_6H_{14}O_6$	dulcitol (c)	−720.68	−321.83	[76, 345, 377, 457, 476, 481]
$C_7H_{16}O_7$	D-perseitol (c)	−835.2	−369.7	[476]
$C_7H_{10}O_7$	D-gluco-α-heptite (c)	−840.4	−364.5	[156]
$C_{10}H_{22}O_2$	1,10-decanediol (c)	−1526.20	−165.78	[343]
$C_{10}H_{22}O_7$	dipentaerythritol (c)	−1315.1	−376.9	[307]
$C_{12}H_{22}O_6$	1,2,5,6-diacetone-mannitol (c)	−1530	−350	[17]

1,2-ethanediol, *(ethylene glycol)* *(liq)* — The combustion data of Parks, West, Naylor, Fujii, and McClaine [345] were preferred for the selected value.

1,2-propanediol *(liq)* — The combustion data of Moureu and Dode [322] were preferred to those of Louguinine [259].

1,2,3-propanetriol, *(glycerol)* *(liq)* — The combustion data of Parks, West, Naylor, Fujii, and McClaine [345] were chosen in preference to the earlier combustion data.

meso-1,2,3,4-butanetetrol, *(meso-erythritol)* *(c)* — The combustion data of Parks, West, Naylor, Fujii, and McClaine [345] were chosen in preference to the earlier combustion data.

pentaerythritol *(c)* — The combustion data of Medard and Thomas [305] were preferred to the data of Stohmann [476].

acetone glycerol *(liq)* — Baer and Flehmig [17] give combustion data for D-, L-, and DL-isomers, but because of their scant description of calorimetric procedures and results, we have assigned a single value to all isomers.

D-mannitol *(c)* — The combustion data of Parks, West, Naylor, Fujii, and McClaine [345] were preferred to any data published before 1900 (references [76, 162, 377, 457, 460, 476, 481]). The recent combustion data of Baer and Flehmig [17] are in poor agreement with our selected value, deviating by 6 to 7 kcal mol^{-1}. Details of their calorimetric procedures and data are scant, and the 6 to 7 kcal mol^{-1} could be the overall uncertainty in their experiments.

dulcitol *(c)* — The combustion data of Parks, West, Naylor, Fujii, and McClaine [345] were chosen in preference to the earlier combustion data.

1,2,5,6-diacetone-mannitol *(c)* — Baer and Flehmig [17] give combustion data for D-, and L-isomers, but because of their scant description of calorimetric procedures and results, we have assigned a single value to both isomers.

6.7. Ethers

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
C_2H_6O	dimethyl ether (g)	−349.06	−43.99	[32, 360, 531]
C_3H_8O	methyl ethyl ether (g)	−503.69	−51.72	[360, 531]
$C_4H_{10}O$	diethyl ether (g)	−657.52	−60.26	[361, 458, 531]
$C_4H_{10}O_2$	1,2-dimethoxyethane (liq)	−627.76	−90.02	[286]

dimethyl ether *(g)* — The combustion data of Pilcher, Pell, and Coleman [360] were preferred to the earlier work.

methyl ethyl ether *(g)* — The combustion data of Pilcher, Pell, and Coleman [360] were preferred to the earlier data of Thomsen [531].

diethyl ether *(g)* — The combustion data of Pilcher, Skinner, Pell, and Pope [361] were preferred to the earlier work.

6.8. Aldehydes

Formula	Compound (State)	$\Delta Hc°$298 K kcal mol^{-1}	$\Delta Hf°$298 K kcal mol^{-1}	Reference
CH_2O	formaldehyde (g) (methanal)	-136.42	-25.95	[558, 591]
$C_2H_2O_2$	glyoxal (g)	-205.76	-50.66	[591]
C_2H_4O	acetaldehyde (g) (ethanal)	-285.01	-39.72	[65, 139]
C_2H_4O	acetaldehyde (liq) (ethanal)	-278.77	-45.96	[49, 50, 105, 406]
C_3H_6O	n-propionaldehyde (liq) (1-propanal)	-434.1	-53.0	[49, 50, 534]
$C_3H_6O_3$	glyceraldehyde (liq)	-344	-143	[17]
C_4H_8O	n-butyraldehyde (liq) (1-butanal)	-592.2	-57.3	[326, 534]
$C_5H_{10}O$	n-valeraldehyde (liq) (1-pentanal)	-742	-70	[262]
$C_5H_{10}O_2$	5-hydroxy-1-pentanal (liq)	-697.1	-114.7	[442]
$C_6H_{10}O_3$	acetone glyceraldehyde (liq)	-726	-180	[17]
$C_6H_{12}O_3$	paraldehyde (liq)	-810.0	-164.2	[90, 155, 265]
C_7H_6O	benzaldehyde (liq)	-843.2	-20.1	[246, 487]
$C_7H_6O_2$	salicylaldehyde (liq)	-796.4	-66.9	[71, 134, 386]
$C_7H_{14}O$	n-heptaldehyde (liq)	-1062.2	-74.4	[261, 326]
$C_8H_{16}O$	n-octaldehyde (liq)	-1218.9	-80.0	[161]

formaldehyde (methanal) (g)—The combustion data of Fletcher and Pilcher [591] were preferred to those of von Wartenberg and Lerner-Steinberg [558].

acetaldehyde (ethanal) (g)—The heat-of-hydrogenation data of Dolliver, Gresham, Kistiakowsky, Smith, and Vaughan [139] were used as the basis of our selected value rather than the early combustion data of Berthelot and Ogier [65].

acetaldehyde (ethanal) (liq)—The heat of vaporization of ethanal as determined by Coleman and DeVries [105], 6.24 kcal mol^{-1} at 25 °C, was combined with the heat of formation of gaseous acetaldehyde. The combustion data of Berthelot and Delepine [49, 50], and Roth and Müller [406] were not used.

n-propionaldehyde (1-propanal) (liq)—The combustion data of Tjebbes [534] were used to obtain the selection. The data of Berthelot and Delepine [49, 50] were not used.

glyceraldehyde (liq)—Baer and Flehmig [17] give combustion data for D-, L-, and DL-isomers, but because of their scant description of calorimetric procedures and results, we have assigned a single value to all isomers.

n-butyraldehyde (1-butanal) (liq)—The combustion data of Tjebbes [534] and Nicholson [326] were averaged to make the selection.

acetone glyceraldehyde (liq)—Baer and Flehmig [17] give combustion data for D-, and L-isomers, but because of their scant description of calorimetric procedures and results, we have assigned a single value to both isomers.

paraldehyde (liq)—The combustion data of Fletcher, Mortimer, and Springall [155] were used to obtain the selected value. The same data are given earlier by Cass, Springall, and White [90], but show $\Delta Hc°$ to be more negative by 0.2 kcal mol^{-1}. The combustion data of Louguinine [265] were not used.

benzaldehyde (liq)—The combustion data of Landrieu, Baylocq, and Johnson [246] were chosen in preference to the data of Stohmann, Rodatz, and Herzberg [487].

salicylaldehyde (liq)—The combustion data of Delepine and Rivals [134] were chosen in preference to the data of Berthelot and Rivals [71] and Rivals [386].

n-heptaldehyde (liq)—The combustion data of Nicholson [326] were chosen in preference to the data of Louguinine [261].

6.9. Ketones

Formula	Compound (State)	$\Delta Hc°$298 K kcal mol^{-1}	$\Delta Hf°$298 K kcal mol^{-1}	Reference
C_3H_6O	propanone (g) (acetone)	-435.32	-51.78	[310, 531]
C_3H_6O	propanone (liq) (acetone)	-427.92	-59.18	[49, 50, 144, 351, 528]
C_4H_8O	butanone (g) (methyl ethyl ketone)	-590.20	-59.26	[123]
C_4H_8O	butanone (liq) (methyl ethyl ketone)	-584.17	-65.29	[317, 344, 378, 436 516]

6.9. Ketones—Continued

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_4H_6O_2$	2,3-butanedione (liq) (diacetyl)	−493.71	−87.44	[245, 327, 341, 449]
$C_5H_{10}O$	2-pentanone (liq) (methyl n-propyl ketone)	−740.78	−71.05	[178, 516, 575]
$C_5H_{10}O$	3-pentanone (liq) (diethyl ketone)	−740.96	−70.87	[178, 264, 406, 516, 575]
C_8H_8O	acetophenone (liq)	−991.60	−34.07	[109, 110, 462, 488]
$C_{13}H_{10}O$	benzophenone (c)	−1556.2	−8.0	[22, 86, 108, 247, 344, 462, 488]

propanone (acetone) (g)—The combustion data of Miles and Hunt [310] were chosen in preference to the early data of Thomsen [531].

propanone (acetone) (liq)—The heat of vaporization was taken from the data of Pennington and Kobe [351], ΔHvap° at 25 °C = 7.40 kcal mol^{-1}. The latter value was combined with the heat of combustion of gaseous propanone. The combustion data of Berthelot and Delepine [49, 50], Emery and Benedict [144], and Taylor, Hall, and Thomas [528] were not used.

butanone (methyl ethyl ketone) (liq)—The combustion data of Sinke and Oetting [436] were chosen in preference to any previous work.

2,3-butanedione (diacetyl) (liq)—The combustion data of Nicholson, Szwarc, and Taylor [327], and Parks, Manchester, and Vaughan [341] were averaged to make the selection. The data of Springall and White [449] and Landrieu [245] were not used.

2-pentanone (methyl n-propyl ketone) (liq)—The combustion data of Harrop Head, and Lewis [178] were preferred to those of Zubov [575] as corrected by Swietoslawski [516].

3-pentanone (diethyl ketone) (liq)—The combustion data of Harrop, Head, and Lewis [178] were preferred to those of Roth and Müller [406], Louguinine [264], and Zubov [575] as corrected by Swietoslawski [516].

acetophenone (liq)—The combustion data of Colomina, Latorre, and Perez-Ossorio [109, 110] were chosen in preference to the early combustion data of Stohmann [462], and Stohmann, Rodatz, and Herzberg [488].

benzophenone (c)—The combustion data of Colomina, Cambeiro, Perez-Ossorio, and Latorre [108], and Parks, Mosley, and Peterson [344] were averaged for the selection. The data of Beckers [22], Burriel [86], Landrieu, and Blatt [247], Stohmann, Rodatz, and Herzberg [488], and Stohmann [462] were not used.

6.10. n-Aliphatic Acids

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
CH_2O_2	formic acid (liq) (methanoic acid)	−60.86	−101.51	[34, 59, 60, 208, 248, 434]
$C_2H_4O_2$	acetic acid (liq) (ethanoic acid)	−209.02	−115.71	[59, 60, 146, 248, 395, 416, 417]
$C_3H_6O_2$	propionic acid (liq) (propanoic acid)	−365.03	−122.07	[248, 265, 417, 472, 473]
$C_4H_8O_2$	butyric acid (liq) (butanoic acid)	−521.87	−127.59	[248, 472, 473]
$C_5H_{10}O_2$	valeric acid (liq) (pentanoic acid)	−678.12	−133.71	[3, 176, 248, 472, 473]
$C_6H_{12}O_2$	caproic acid (liq) (hexanoic acid)	−834.49	−139.71	[3, 152, 248, 263]
$C_7H_{14}O_2$	enanthic acid (liq) (heptanoic acid)	−990.81	−145.75	[3, 248]
$C_8H_{16}O_2$	caprylic acid (liq) (octanoic acid)	−1147.00	−151.93	[3, 248, 266, 267]
$C_9H_{18}O_2$	pelargonic acid (liq) (nonanoic acid)	−1303.62	−157.67	[3, 248, 266, 267, 472, 473]
$C_{10}H_{20}O_2$	capric acid (liq) (decanoic acid)	−1460.1	−163.6	[2, 3]
$C_{10}H_{20}O_2$	capric acid (c) (decanoic acid)	−1453.07	−170.59	[3, 457, 472, 473, 481]

6.10. n-Aliphatic Acids—Continued

Formula	Compound (State)	$\Delta Hc°298\,K$ kcal mol^{-1}	$\Delta H f°298\,K$ kcal mol^{-1}	Reference
$C_{12}H_{24}O_2$	lauric acid (liq) (dodecanoic acid)	−1772.0	−176.4	[2, 3]
$C_{12}H_{24}O_2$	lauric acid (c) (dodecanoic acid)	−1763.25	−185.14	[3, 176, 266, 267, 409, 474, 482]
$C_{14}H_{28}O_2$	myristic acid (liq) (tetradecanoic acid)	−2084.6	−188.5	[2, 3]
$C_{14}H_{28}O_2$	myristic acid (c) (tetradecanoic acid)	−2073.91	−199.21	[3, 266, 267, 377, 457, 474, 481, 482, 506]
$C_{16}H_{32}O_2$	palmitic acid (liq) (hexadecanoic acid)	−2397.5	−200.4	[2, 3, 176, 248]
$C_{16}H_{32}O_2$	palmitic acid (c) (hexadecanoic acid)	−2384.76	−213.10	[3, 144, 266, 267, 457, 472, 473, 506]
$C_{18}H_{36}O_2$	stearic acid (liq) (octadecanoic acid)	−2710.1	−212.5	[2, 3, 248]
$C_{18}H_{36}O_2$	stearic acid (c) (octadecanoic acid)	−2696.12	−226.47	[3, 144, 248, 266, 303, 377, 410, 457, 472, 473, 481, 506]
$C_{20}H_{40}O_2$	arachidic acid (liq) (eicosanoic acid)	−3022.7	−224.6	[2, 3]
$C_{20}H_{40}O_2$	arachidic acid (c) (eicosanoic acid)	−3005.50	−241.82	[3, 472, 433]
$C_{22}H_{44}O_2$	behenic acid (c) (docosanoic acid)	−3337	−235	[474]

formic acid, (methanoic acid) *(liq)*—The combustion data of Sinke [434] were used to obtain the selected value. The data of Lebedeva [248] are *in excellent* agreement with the selection. The data of Berthelot [34], Berthelot and Matignon [59, 60], and Jahn [208] were not used.

acetic acid, (ethanoic acid) *(liq)*—The combustion data of Evans and Skinner [146] were used to obtain the selected value. The data of Lebedeva [248] are in excellent agreement with the selection. The data of Berthelot and Matignon [59, 60], Roth [395], and Schjånberg [416, 417] were not used, although only the data of Roth [395] appeared to deviate from the selection by more than 0.3 kcal mol^{-1}.

propionic acid, (propanoic acid) *(liq)*—The combustion data of Lebedeva [248] were chosen in preference to the previous data.

n-butyric acid, (n-butanoic acid) *(liq)*—The combustion data of Lebedeva [248] were chosen in preference to the early data.

n-valeric acid, (n-pentanoic acid) *(liq)*—The combustion data of Lebedeva [248], and Adriaanse, Dekker, and Coops [3] were averaged to obtain the selected value. The data of Hancock, Watson, and Gilby [176] agree well with the early work of Stohmann, Kleber, Langbein, and Offenhauer [472, 473]. Data from the latter three references were not used.

n-caproic acid, (n-hexanoic acid) *(liq)*—The combustion data of Lebedeva [248], and Adriaanse, Dekker, and Coops [3] were averaged to obtain the selected value. The data of Fischer and Wrede [152], and Louguinine [263] were not used.

enanthic acid, (n-heptanoic acid) *(liq)*—The combustion data of Lebedeva [248], and Adriaanse, Dekker, and Coops [3] were averaged to obtain the selection.

caprylic acid, (n-octanoic acid) *(liq)*—The combustion

data of Lebedeva [248] and Adriaanse, Dekker, and Coops [3] were averaged to obtain the selected value. The data of Louguinine [266, 267] were not used.

pelargonic acid, (n-nonanoic acid) *(liq)*—The combustion data of Lebedeva [248], and Adriaanse, Dekker, and Coops [3] were averaged to obtain the selection. The early data were not used.

capric acid, (n-decanoic acid) *(c)*—The combustion data of Adriaanse, Dekker, and Coops [3] were chosen in preference to the earlier data.

lauric acid, (n-dodecanoic acid) *(c)*—The combustion data of Adriaanse, Dekker, and Coops [3] were chosen in preference to the earlier data.

myristic acid (n-tetradecanoic acid) *(c)*—The combustion data of Adriaanse, Dekker, and Coops [3] were used to obtain the selected value. The data of Swain, Silbert, and Miller [506], although not as precise, are in good agreement with the selection. The early combustion data were not used.

palmitic acid, (n-hexadecanoic acid) *(liq)*—The heat of fusion as determined by Adriaanse, Dekker, and Coops [2, 3] was selected in preference to that of Lebedeva [248] and combined with the combustion data on the crystal.

palmitic acid, (n-hexadecanoic acid) *(c)*—The combustion data of Adriaanse, Dekker, and Coops [3] were used to obtain the selected value in preference to the data of Lebedeva [248]. The data of Swain, Silbert, and Miller [506], although not as precise as either of the above data are in good agreement with the data of Adriaanse, Dekker, and Coops [3]. Data prior to the above were not used.

stearic acid, (n-octadecanoic acid) *(liq)*—The fusion data of Lebedeva [248], and Adriaanse, Dekker, and Coops [2, 3] were averaged to obtain the selected value, ΔH(fusion) at 25 °C = 14.0 kcal mol^{-1} and

combined with the combustion data on the crystal.
stearic acid, (n-octadecanoic acid) (c)—The combustion data of Lebedeva [248], and Adriaanse, Dekker, and Coops [3] were averaged to obtain the selected value. The combustion data of Swain, Silbert, and Miller

[506] are too positive by about 2.2 kcal mol^{-1}. Data prior to the above were not used.
arachidic acid, (n-eicosanoic acid) (c)—The combustion data of Adriaanse, Dekker, and Coops [3] were preferred to the earlier work.

6.11. Hydroxy and Keto Aliphatic Acids

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_2H_4O_3$	glycolic acid (c) (hydroxyacetic acid)	-166.1	-158.6	[271, 460]
$C_2H_4O_4$	glyoxylic acid (c)	-125.0	-199.7	[34, 61]
$C_3H_4O_3$	pyruvic acid (c)	-278.5	-140.3	[79]
$C_3H_4O_6$	mesoxalic acid (c)	-128.1	-290.7	[294]
$C_3H_6O_3$	D-lactic acid (c)	-321.22	-165.88	[415]
$C_3H_6O_3$	DL-lactic acid (liq)	-326.8	-160.3	[144, 271]
$C_4H_8O_3$	DL-β-hydroxybutyric acid (liq)	-487.2	-162.3	[144]
$C_4H_8O_3$	hydroxyisobutyric acid (c)	-471.6	-177.9	[269, 271]
$C_5H_8O_3$	levulinic acid (c) (γ-ketovaleric acid)	-576.9	-166.6	[44]
$C_6H_{12}O_7$	D-galactonic acid (c)	589.4	-384.8	[497]
$C_6H_{12}O_7$	D-gluconic acid (c)	-594.9	-379.3	[497]
$C_{22}H_{44}O_4$	13,14-dihydroxybehenic acid (c)	-3235	-337	[474]

glycolic acid, (hydroxyacetic acid) (c)—The combustion data of Louguinine [271], and Stohmann [460] were averaged to obtain the selected value.

glyoxylic acid (c)—The combustion data of Berthelot [34] are the same as Berthelot and Matignon [61].

DL-lactic acid (liq)—The combustion data of Emery and Benedict [144] and Louguinine [271] were averaged to obtain the selected value.

hydroxyisobutyric acid (c)—The later combustion data of Louguinine [271] were preferred to the earlier work by the same author [269].

6.12. Unsaturated Aliphatic Acids

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_3H_4O_2$	acrylic acid (liq)	-327.0	-91.8	[321, 385]
$C_4H_6O_2$	*cis*-crotonic acid (liq)	-498	-83	[99]
$C_4H_6O_2$	*trans*-crotonic acid (c)	-478.2	-102.9	[462]
$C_5H_8O_2$	angelic acid (c) (*trans*-α,β-dimethylacrylic acid)	-634.6	-108.9	[461, 462]
$C_5H_8O_2$	tiglic acid (c) (*cis*-α,β-dimethylacrylic acid)	-626.2	-117.3	[461, 462]
$C_6H_8O_2$	sorbic acid (c)	-744.2	-93.4	[152, 333, 462]
$C_6H_{10}O_2$	hydrosorbic acid (liq)	-795.7	-110.2	[152]
$C_{11}H_{20}O_2$	undecyl-10-ene-1-oic acid (c)	-1580	-138	[462]
$C_{18}H_{34}O_2$	elaidic acid (c)	-2636.6	-217.7	[222, 223, 462]
$C_{18}H_{34}O_2$	oleic acid (liq)	-2675.4	-178.9	[223]
$C_{18}H_{34}O_2$	oleic acid (c)	-2667.1	-187.2	[144, 222, 223, 229, 462]
$C_{22}H_{42}O_2$	brassidic acid (c)	-3290	-214	[461, 474]
$C_{22}H_{42}O_2$	erucic acid (c)	-3297	-207	[461, 474]

acrylic acid (liq)—The combustion data of Moureu and Boutaric [321], and Riiber and Schetelig [385] were averaged to obtain the selected value.
tiglic acid (cis-α, β-dimethylacrylic acid) (c)—The combustion data of Stohmann [461] and Stohmann [462] are the same.
angelic acid (trans-α, β-dimethylacrylic acid) (c)—The combustion data of Stohmann [461] and Stohmann [462]

are the same.
sorbic acid (c)—The combustion data of Fischer and Wrede [152] were chosen in preference to the data of Stohmann [462] and Ossipov [333].
oleic acid (c)—The combustion data of Keffler and McLean [229] were chosen for the selected value. The earlier data of Keffler [222, 223] are in good agreement with the selection.

elaidic acid (*c*)—The combustion data of Keffler [222, 223] were chosen in preference to the data of Stohmann [462].

erucic acid (*c*)—The combustion data of Stohmann and Langbein [474] are the same as Stohmann [461].
brassidic acid (*c*)—The combustion data of Stohmann and Langbein [474] are the same as Stohmann [461].

6.13. Aliphatic Dicarboxylic Acids

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_2H_2O_4$	oxalic acid (c, α)	−58.7	−197.7	[19, 208, 348, 377, 457, 470, 481, 550, 564]
$C_2H_2O_4$	oxalic acid (c, β)	−59.0	−197.4	[527]
$C_2H_6O_6$	oxalic acid dihydrate (c)	−52.0	−341.0	[19, 214, 215]
$C_3H_4O_4$	malonic acid (c)	−205.82	−212.96	[269, 271, 377, 457, 470, 550, 564]
$C_4H_6O_4$	succinic acid (c)	−356.36	−224.79	[22, 84, 89, 193, 226, 232, 269, 271, 314, 362, 377, 396, 401, 441, 457, 470, 481, 524, 550, 564, 592, 593, 594, 595, 596]
$C_5H_8O_4$	glutaric acid (c)	−514.08	−229.44	[467, 470, 550, 564]
$C_6H_{10}O_4$	adipic acid (c)	−668.29	−237.60	[470, 550]

α-oxalic acid (*c*)—The combustion data of Becker and Roth [19] on oxalic acid dihydrate were combined with their data on the heats of solution of anhydrous α-oxalic acid and oxalic acid dihydrate to obtain the selected value for the heat of combustion of α-oxalic acid. The combustion data of Wilhoit and Shaio [564] are in reasonable agreement with the selection.
β-oxalic acid (*c*)—The data of Taylor [527] on the heats of solution of α- and β-oxalic acids were combined with the heat of combustion of α-oxalic acid to obtain the selected value.
oxalic acid dihydrate (*c*)—The combustion data of Becker and Roth [19] were preferred to that of Jorissen and van de Stadt [214, 215].
malonic acid (*c*)—The combustion data of Wilhoit and Shaio [564] were used to make the selection. Agreement with the data of Verkade, Hartman, and

Coops [550] is good.
succinic acid (*c*)—The combustion data of Keith and Mackle [232], Pilcher and Sutton [362], Cass, Springall, and Quincey [89], Huffman [193], Adams, Carson, and Laye [592], Bills and Cotton [593], Ducros, Levy, and Meliava [594], Good, et al. [596], and Wilhoit and Shaio [564] were averaged to obtain the selected value. The data of any of the above authors differ from the selected value by less than 0.1 kcal mol^{-1}.
glutaric acid (*c*)—The combustion data of Wilhoit and Shaio [564] were used to obtain the selection. Agreement with the data of Verkade, Hartman and Coops [550] is good.
adipic acid (*c*)—The combustion data of Verkade, Hartman, and Coops [550] were used to make the selection, although agreement with the data of Stohmann, Kleber and Langbein [470] is good.

6.14. Hydroxy and Keto Aliphatic Dicarboxylic Acids

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_4H_6O_5$	L-malic acid (c)	−317.37	−263.78	[564]
$C_4H_6O_5$	DL-malic acid (c)	−316.88	−264.27	[564]
$C_4H_6O_6$	L-tartaric acid (c)	−274.7	−306.5	[78, 116, 142, 377 457, 481]
$C_4H_6O_6$	DL-tartaric acid (c)	−272.6	−308.5	[78, 116, 142, 335, 337, 338]
$C_4H_6O_6$	meso-tartaric acid (c)	−275.3	−305.9	[78, 116, 142]
$C_4H_8O_7$	DL-tartaric acid monohydrate (c)	−278	−371	[335, 337, 338]
$C_5H_6O_5$	α-ketoglutaric acid (c)	−429.85	−245.35	[563]
$C_5H_8O_7$	DL-trihydroxyglutaric acid (c)	−388	−356	[156]
$C_6H_8O_7$	citric acid (anhydrous) (c)	−468.6	−369.0	[271, 377, 457, 470, 470, 481, 564]
$C_6H_{10}O_8$	citric acid monohydrate (c)	−466.48	−439.40	[93, 271]
$C_6H_{10}O_8$	allomucic acid (c)	−494	−412	[156]
$C_6H_{10}O_8$	mucic acid (c)	−483	−423	[462]

L-tartaric acid (c)—The combustion data of Coops and Verkade [116] were chosen.

DL-tartaric acid (c)—The combustion data of Coops and Verkade [116] were chosen.

meso-tartaric acid (c)—The combustion data of Coops and Verkade [116] were chosen.

DL-tartaric acid monohydrate (c)—The later combus-

tion data of Ossipov [337, 338] were preferred to the earlier data [335].

citric acid (*anhydrous*) (c)—The combustion data of Wilhoit and Shaio [564] were used.

citric acid monohydrate (c)—The combustion data of Chappel and Hoare [93] were used.

6.15. Unsaturated Aliphatic Dicarboxylic Acids

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_4H_4O_4$	maleic acid (c)	−323.89	−188.94	[199, 257, 268, 271, 339, 422, 470, 564]
$C_4H_4O_4$	fumaric acid (c)	−318.99	−193.84	[199, 257, 268, 271, 339, 422, 459, 476, 564]
$C_5H_6O_4$	citraconic acid (c)	−478.16	−197.04	[268, 271, 461, 462, 563]
$C_5H_6O_4$	itaconic acid (c)	−474.14	−201.06	[268, 271, 462, 563]
$C_5H_6O_4$	mesaconic acid (c)	−478	−197	[268, 271]
$C_6H_6O_6$	*cis*-aconitic acid (c)	−476.6	−292.7	[271, 462, 563]
$C_6H_6O_6$	*trans*-aconitic acid (c)	−474.6	−294.7	[271, 462, 563]
$C_6H_8O_4$	hexa-2-ene-1,6-dioic acid (c)	−629	−209	[462]
$C_6H_8O_4$	hexa-3-ene-1,6-dioic acid (c)	−629	−209	[462]
$C_7H_{10}O_4$	tetraconic acid (c)	−796	−204	[336, 337, 338]

maleic acid (c)—The combustion data of Wilhoit and Shaio [564] were chosen for the selected value. The data of Schwabe and Wagner [422], and Huffman and Fox [199] are in good agreement with the selection.

fumaric acid (c)—The combustion data of Wilhoit and Shaio [564] were chosen for the selected value. The data of Schwabe and Wagner [422], and Huffman and Fox [199] are in good agreement with the selection.

citraconic acid (c)—The combustion data of Wilhoit and Lei [563] were used.

itaconic acid (c)—The combustion data of Wilhoit and Lei [563] were used.

mesaconic acid (c)—The later combustion data of Louguinine [271] were preferred to the earlier work [268].

cis- and trans-aconitic acids (c)—The combustion data of Wilhoit and Lei [563] were used.

tetraconic acid (c)—The combustion data of Ossipov [336, 337, 338] are the same.

6.16. Aromatic Acids and Phenylated Aliphatic Acids

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_7H_6O_2$	benzoic acid (c)	−771.27	−92.03	[57, 70, 91, 95, 112, 138, 152, 153, 154, 171, 173, 182, 205, 210, 211, 212, 246, 277, 278, 309, 319, 332, 352, 374, 377, 395, 402, 457, 469, 481, 487, 514, 515, 517, 518, 519, 521, 522, 571, 582]
$C_7H_6O_3$	salicylic acid (c)	−722.4	−140.9	[21, 28, 30, 102, 103, 134, 221, 224, 225, 228, 313, 377, 403, 457, 469, 480, 539, 541, 542, 544]
$C_8H_6O_3$	phenylglyoxylic acid (c)	−842.1	−115.3	[325]
$C_8H_6O_4$	*o*-phthalic acid (c)	−770.44	−186.91	[271, 377, 384, 423, 457, 462, 469, 548]
$C_8H_6O_4$	*m*-phthalic acid (c)	−765.44	−191.91	[423, 469, 548]

6.16.   Aromatic Acids and Phenylated Aliphatic Acids—Continued

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_8H_6O_4$	p-phthalic acid (c)	−762.30	−195.05	[423, 469]
$C_8H_8O_2$	phenylacetic acid (c)	−930.4	−95.3	[13, 152, 377, 460, 469, 492, 571]
$C_8H_8O_3$	L-mandelic acid (c)	−886.9	−138.8	[460, 480, 574]
$C_8H_8O_3$	DL-mandelic acid (c)	−887.2	−138.5	[460, 480, 574]
$C_8H_8O_3$	phenoxyacetic acid (c)	−902.9	−122.8	[460, 480]
$C_9H_{10}O_4$	DL-phenylglyceric acid (c)	−1009.5	−178.5	[27]

benzoic acid (*c*)—The selected value was obtained by using $\Delta U_B = -26434$ J g^{-1} at 25 °C [579], and applying the corrections for standard states and ΔnRT. Recent assessments and redeterminations of the heat of combustion of benzoic acid with respect to its use as a primary thermochemical standard for the calibration of bomb calorimeters can be found in the papers by Churney and Armstrong [95], Gundry, Harrop, Head, and Lewis [171], and Mosselman and Dekker [319]. The references cited give a chronological evolution of the use of benzoic acid as a standard in combustion bomb calorimetry.

salicylic acid (*c*)—The combustion data of Verkade [539], Verkade and Coops [544], and Keffler [225] were combined to make the selection. The data of Beckers are in good agreement with the selection.

o-phthalic acid (*c*)—The combustion data of Schwabe and Wagner [423] were used to make the selection. The data of Richardson and Parks [384] are in good agreement with the selection.

m-phthalic acid (*c*)—The combustion data of Schwabe and Wagner [423] were used to obtain the selected value.

p-phthalic acid (*c*)—The combustion data of Schwabe and Wagner [423] were used to obtain the selected value.

phenylacetic acid (*c*)—The combustion data of von Auwers and Roth [13], and Wrede [571] were averaged to obtain the selected value.

L- and DL-mandelic acid (*c*)—The combustion data of Zubareva et al. [574] were used in preference to the earlier work.

6.17.   Acid Anhydrides

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_4H_2O_3$	maleic anhydride (c)	−332.10	−112.42	[271, 336, 337, 338, 344, 564]
$C_4H_4O_3$	succinic anhydride (c)	−369.0	−143.8	[271, 460, 549]
$C_4H_6O_3$	acetic anhydride (liq)	−431.70	−149.45	[395, 554]

maleic anhydride (*c*)—The combustion data of Wilhoit and Shaio [564] were used. The data of Parks, Mosley, and Peterson [344] are in good agreement with the selected value.

succinic anhydride (*c*)—The combustion data of Ver-

kade and Hartman [549] were used to obtain the selection.

acetic anhydride (*liq*)—The aminolysis data of Wadsö [554] were used in preference to the combustion data of Roth [395].

6.18.   Methyl Esters of Monobasic Aliphatic Acids

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_2H_4O_2$	methyl formate (g)	−241.0	−83.7	[66, 531]
$C_2H_4O_2$	methyl formate (liq)	−234.1	−90.6	[49, 50, 150, 398]
$C_3H_6O_2$	methyl acetate (liq)	−380.7	−106.4	[407]
$C_6H_{12}O_2$	methyl valerate (liq)	−851.31	−122.89	[3, 176]
$C_7H_{14}O_2$	methyl caproate (liq)	−1007.46	−129.10	[3]
$C_8H_{16}O_2$	methyl enanthate (liq)	−1163.40	−135.53	[3]
$C_9H_{18}O_2$	methyl caprylate (liq)	−1320.22	−141.07	[3]
$C_{10}H_{20}O_2$	methyl pelargonate (liq)	−1476.37	−147.29	[3]
$C_{11}H_{22}O_2$	methyl caprate (liq)	−1632.96	−153.07	[3]
$C_{12}H_{24}O_2$	methyl undecylate (liq)	−1789.42	−158.97	[3]
$C_{13}H_{26}O_2$	methyl laurate (liq)	−1945.10	−165.66	[3]
$C_{14}H_{28}O_2$	methyl tridecylate (liq)	−2101.56	−171.56	[3]
$C_{15}H_{30}O_2$	methyl myristate (liq)	−2257.69	−177.80	[3]
$C_{16}H_{32}O_2$	methyl pentadecylate (liq)	−2413.51	−184.35	[3]
$C_{19}H_{36}O_2$	methyl oleate (liq)	−2842.4	−174.2	[222, 227, 229]
$C_{19}H_{36}O_2$	methyl elaidate (liq)	−2840.8	−175.8	[222, 227]

The combustion data of Adriaanse, Dekker, and Coops [3] were adjusted to the 1961 atomic mass scale because the data were based upon the moles of ester introduced into the bomb prior to an experiment calculated on an earlier atomic mass scale.

methyl formate (g) — The combustion data of Thomsen [531] were used in preference to that of Berthelot and Ogier [66].

methyl formate (liq) — The combustion data of Berthelot and Delepine [49, 50] and Roth and Banse [398] were combined to obtain the selected value.

methyl valerate (liq) — The combustion data of Adriaanse, Dekker, and Coops [3] were used to obtain the selected value.

methyl oleate (liq) — The later combustion data of Keffler [227], and Keffler and McLean [229] were used to obtain the selected value.

methyl elaidate (liq) — The later combustion data of Keffler [227] were used to make the selection.

6.19. Methyl Esters of Monobasic Aromatic Acids

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol⁻¹	$\Delta Hf°298$ K kcal mol⁻¹	Reference
$C_8H_8O_2$	methyl benzoate (liq)	−945.9	−79.8	[487]
$C_8H_9O_3$	methyl salicylate (liq)	−898.6	−127.1	[435, 488]

methyl salicylate (liq) — The combustion data of Sinke [435] were preferred to those of Stohmann, Rodatz, and Herzberg [488].

6.20. Dimethyl Esters of Dibasic Aliphatic Acids

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol⁻¹	$\Delta Hf°298$ K kcal mol⁻¹	Reference
$C_4H_6O_4$	dimethyl oxalate (liq)	− 400.2	− 181.0	[471, 547]
$C_5H_8O_4$	dimethyl malonate (liq)	− 553.3	− 190.2	[170, 547]
$C_6H_8O_4$	dimethyl maleate (liq)	− 669.4	− 168.2	[336, 337, 338]
$C_6H_8O_4$	dimethyl fumarate (liq)	− 663.3	− 174.3	[336, 337, 338, 471]
$C_6H_{10}O_4$	dimethyl succinate (liq)	− 706.3	− 199.6	[471, 547]
$C_7H_{12}O_4$	dimethyl glutarate (liq)	− 862.3	− 205.9	[547]
$C_8H_{14}O_4$	dimethyl adipate (liq)	− 1018.7	− 211.9	[547]

dimethyl oxalate (liq) — The combustion data of Verkade, Coops, and Hartman [547] were preferred to those of Stohmann, Kleber, and Langbein [471].

dimethyl malonate (liq) — The combustion data of Verkade, Coops, and Hartman [547] were preferred to those of Guinchant [170].

dimethyl fumarate (liq) — The combustion data of Stohmann, Kleber, and Langbein [471] and Ossipov [336, 337, 338] were averaged to obtain the selection.

dimethyl succinate (liq) — The combustion data of Verkade, Coops, and Hartman [547] were preferred to those of Stohmann, Kleber, and Langbein [471].

6.21. Dimethyl Esters of Dibasic Aromatic Acids

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol⁻¹	$\Delta Hf°298$ K kcal mol⁻¹	Reference
$C_{10}H_{10}O_4$	dimethyl o-phthalate (liq)	− 1120	− 162	[471]
$C_{10}H_{10}O_4$	dimethyl m-phthalate (c)	− 1111	− 171	[471]
$C_{10}H_{10}O_4$	dimethyl p-phthalate (c)	− 1112	− 170	[471, 460]

6.22. Glyceryl Esters

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol⁻¹	$\Delta Hf°298$ K kcal mol⁻¹	Reference
$C_5H_{10}O_4$	glyceryl-1-acetate (liq)	−594.3	−217.5	[525]
$C_7H_{12}O_5$	glyceryl-1,3-diacetate (liq)	−800.0	−268.2	[525]
$C_9H_{14}O_6$	glyceryl triacetate (liq)	−1006.4	− 318.3	[525]
$C_{10}H_{12}O_4$	glyceryl-1-benzoate (c)	−1164.61	−185.80	[432]

6.22. Glyceryl Esters—Continued

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_{10}H_{12}O_4$	glyceryl-2-benzoate (c)	−1165.69	−184.71	[432]
$C_{13}H_{26}O_4$	glyceryl-1-caprate (c)	−1845.71	−265.05	[432]
$C_{13}H_{26}O_4$	glyceryl-2-caprate (c)	−1848.87	−261.90	[432]
$C_{15}H_{20}O_6$	tricyclobutyrin (liq)	−1847	−247	[516]
$C_{15}H_{26}O_6$	glyceryl tributyrate (liq)	−1943	−356	[516]
$C_{15}H_{30}O_4$	glyceryl-1-laurate (c)	−2158.03	−277.46	[432]
$C_{15}H_{30}O_4$	glyceryl-2-laurate (c)	−2160.02	−275.48	[432]
$C_{17}H_{34}O_4$	glyceryl-1-myristate (c)	−2467.92	−292.31	[97, 432]
$C_{17}H_{34}O_4$	glyceryl-2-myristate (c)	−2470.34	−289.89	[432]
$C_{18}H_{26}O_6$	tricyclovalerin (liq)	−2311	−270	[516]
$C_{19}H_{38}O_4$	glyceryl-1-palmitate (c)	−2778.67	−306.28	[97, 432]
$C_{19}H_{38}O_4$	glyceryl-2-palmitate (c)	−2781.72	−303.23	[97, 432]
$C_{21}H_{42}O_4$	glyceryl-1-stearate (c)	−3090.05	−319.64	[17, 432]
$C_{21}H_{42}O_4$	glyceryl-2-stearate (c)	−3093.89	−315.80	[432]
$C_{24}H_{20}O_6$	glyceryl tribenzoate (c)	−2726	−214	[488]
$C_{39}H_{74}O_6$	glyceryl trilaurate (c)	−5707	−489	[266, 267, 474]
$C_{45}H_{86}O_6$	glyceryl trimyristate (c)	−6650	−520	[266, 267, 457, 474]
$C_{47}H_{88}O_5$	glyceryl dierucate (c)	−6979	−447	[474]
$C_{47}H_{88}O_5$	glyceryl dibrassidate (c)	−6954	−472	[474]
$C_{69}H_{128}O_6$	glyceryl trierucate (c)	−10266	−596	[474]
$C_{69}H_{128}O_6$	glyceryl tribrassidate (c)	−10237	−625	[474]

The combustion data on the glyceryl esters are given to a decimal place more than their uncertainties would allow in most cases.

glyceryl-1-myristate (c)—The combustion data of Silbert, Daubert, and Mason [432] were chosen in preference to the data of Clarke and Stegeman [97].

glyceryl-1-palmitate (c)—The combustion data of Silbert, Daubert, and Mason [432] were chosen in preference to the data of Clarke and Stegeman [97].

glyceryl-2-palmitate (c)—The combustion data of Silbert, Daubert, and Mason [432] were chosen in

preference to the data of Clarke and Stegeman [97].

glyceryl-1-stearate (c)—The combustion data of Silbert, Daubert, and Mason [432] were preferred to those of Baer and Flehmig [17].

glyceryl trilaurate (c)—The combustion data of Louguinine [266, 267] and Stohmann and Langbein [474] were averaged to give the selected value.

glyceryl trimyristate (c)—The combustion data of Stohmann and Langbein [474] were used for the selected value in preference to the data of Louguinine [266, 267] and Stohmann [457].

6.23. Steroids

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_{19}H_{32}$	5α-androstane (c)	−2805	−75	[340]
$C_{19}H_{26}O_2$	Δ4-androstene-3,17-dione (c)	−2572	−103	[340]
$C_{19}H_{28}O_2$	5α-androstane-3,17-dione (c)	−2613	−130	[340]
$C_{19}H_{28}O_2$	Δ4-androstene-3-one-17β-ol (c) (testosterone)	−2649	−94	[340]
$C_{19}H_{28}O_2$	Δ5-androstene-3β-ol-17-one (c) (trans-dehydroandro-sterone)	−2636	−107	[340]
$C_{19}H_{30}O_2$	5α-androstane-3α-ol-17-one (c) (androsterone)	−2650	−162	[340]
$C_{19}H_{30}O_2$	5α-androstane-3β-ol-17-one (c) (epiandrosterone)	−2660	−152	[340]
$C_{19}H_{30}O_2$	5α-androstane-3-one-17β-ol (c)	−2692	−120	[340]
$C_{21}H_{28}O_5$	Δ4-pregnene-3,11,20-trione-17α,21-diol (c) (cortisone)	−2676	−255	[340]

6.23. Steroids—Continued

Formula	Compound (State)	$\Delta Hc°298\,K$ kcal mol^{-1}	$\Delta Hf°298\,K$ kcal mol^{-1}	Reference
$C_{21}H_{30}O_2$	Δ_4-pregnene-3,20-dione (c) (progesterone)	-2868	-132	[340]
$C_{21}H_{30}O_3$	Δ_4-pregnene-3,20-dione-21-ol (c) (desoxycorticosterone or cortexone)	-2876	-124	[340]
$C_{21}H_{30}O_5$	Δ_4-pregnene-3,20-dione-11β, 17α,21-triol (c) (cortisol)	-2744	-256	[340]
$C_{24}H_{42}O_6$	5β-cholan-24-oic acid-3α,7α, 12α-triol monohydrate (c)	-3404	-288	[35, 37]
$C_{27}H_{46}O$	Δ_5-cholestene-3β-ol (c) (cholesterol)	-3978	-133	[45, 46, 340, 583]
$C_{28}H_{48}O$	Δ_5-cholestene-3β-yl methyl ether (c)	-4117.1	-155.9	[207]
$C_{28}H_{48}O$	3:5-cyclocholestan-6β-yl methyl ether (c)	-4122.8	-150.3	[207]

5α-androstane-3-one-17β-ol (c)—The heat of combustion reported by Paoli et al. [340] is 170 kcal mol^{-1} less negative than the value we cite. The value we selected was obtained by an energy-structure correlation which appeared to be more consistent with the other combustion data on the steroids. Paoli et al. [340], also have reservations on the reliability of their experimental combustion value for this compound.

Δ_4-pregnene-3,20-dione-21-ol (*desoxycorticosterone* or

cortexone) (c)—The combustion data appears more negative than expected when compared to the combustion data on Δ_4-pregnene-3,20-dione. Usually the addition of an OH group makes the heat of combustion more positive by 40 to 50 kcal mol^{-1}.

Δ_5-cholestene-3β-ol (*cholesterol*) (c)—The selection was obtained by averaging the data of Paoli, Garrigues, and Patin [340], Bills, Cox, and Steel [583], and Berthelot and Andre [45, 46].

6.24. Lactones

Formula	Compound (State)	$\Delta Hc°298\,K$ kcal mol^{-1}	$\Delta Hf°298\,K$ kcal mol^{-1}	Reference
$C_3H_4O_2$	β-propiolactone (g)	-351.17	-67.61	[80]
$C_3H_4O_2$	β-propiolactone (liq)	-339.93	-78.85	[80]
$C_4H_4O_2$	β-methylene-β-propiolactone (liq) (diketene)	-457.11	-55.72	[281]
$C_5H_6O_2$	levulinic lactone (liq)	-599.0	-76.2	[44]
$C_5H_8O_5$	D-arabonic acid-γ-lactone (c)	-505.3	-238.2	[497]
$C_6H_6O_6$	D-mannonic-1,4-3,6-dilactone (c)	-514.7	-254.6	[497]
$C_6H_8O_4$	lactide (c)	-653.4	-184.2	[47, 48]
$C_6H_8O_6$	L-ascorbic acid (c)	-559.23	-278.34	[136]
$C_6H_8O_7$	D-glucaric acid-1,4-lactone (c)	-494.4	-343.2	[497]
$C_6H_8O_7$	D-glucaric acid-3,6-lactone (c)	-494.0	-343.6	[497]
$C_6H_{10}O_5$	saccharinic acid lactone (c)	-656.3	-249.6	[463]
$C_6H_{10}O_6$	D-mannonic acid-γ-lactone (c)	-609.7	-296.2	[156, 497]
$C_6H_{10}O_6$	D-galactonic acid-γ-lactone (c)	-607.6	-298.3	[497]
$C_6H_{10}O_6$	L-gulonic acid-γ-lactone (c)	-614.4	-291.5	[156]
$C_6H_{10}O_6$	D-gluconic acid-δ-lactone (c)	-605.6	-300.3	[497]
$C_7H_{10}O_4$	terebic acid (c)	-778	-222	[333, 334, 337, 338]
$C_7H_{12}O_7$	D-gluco-D-gulo-heptonic acid-γ-lactone (c)	-712.7	-355.6	[156, 497]
$C_8H_{14}O_8$	D-gluco-α,α-octonic acid-γ-lactone (c)	-836.4	-394.2	[156]
$C_{10}H_{16}O_2$	dehydro-β-campholeno-lactone (c) (inactive)	-1350	-137	[72]
$C_{10}H_{16}O_2$	dehydro-β-campholeno-lactone (c) (dextrorotatory)	-1357	-130	[72]

6.24. Lactones—Continued

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_{10}H_{16}O_3$	methyl ethyl heptanone lactone (c) (racemic)	−1303.5	−183.5	[177]
$C_{12}H_{18}O_2$	3(a)-hydroxy-trans-decalin-2(a) acetic acid lactone (c)	−1610.36	−133.09	[159]
$C_{12}H_{18}O_2$	3(e)-hydroxy-trans-decalin-2(e) acetic acid lactone (c)	−1606.19	−137.26	[159]

D-mannonic acid-γ-lactone (c)—The combustion data of Stroh and Küchenmeister [497] were used for the selection. The early combustion data of Fogh [156] were not used.
terebic acid (c)—The early combustion data of Ossipov

[333, 334] were not used. The selection was made from the later publications [337, 338].
D-gluco-D-gulo-heptonic acid-γ-lactone (c)—The combustion data of Stroh and Küchenmeister [497] were preferred to those of Fogh [156].

6.25. Monosaccharides

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_5H_{10}O_5$	α-D-xylose (c)	−559.0	−252.8	[58, 220, 442]
$C_5H_{10}O_5$	β-D- and β-L-arabinose (c)	−558.99	−252.84	[58, 136, 220, 457, 476, 481]
$C_5H_{10}O_5$	β-D-ribose (c)	−560.67	−251.16	[136, 496]
$C_6H_{10}O_5$	levoglucosan (c)	−676.6	−229.3	[220, 418, 442]
$C_6H_{12}O_5$	D-fucose (c)	−711.5	−262.7	[476]
$C_6H_{12}O_5$	β-L-rhamnose (c)	−717.7	−256.5	[220, 476]
$C_6H_{12}O_6$	α-D-glucose (c)	−669.94	−304.26	[70, 144, 162, 199, 366, 369, 377, 442, 457, 460, 470, 481]
$C_6H_{12}O_6$	β-D-glucose (c)	−671.44	−302.76	[180, 181, 199, 498, 529]
$C_6H_{12}O_6$	α-D-galactose (c)	−670.1	−304.1	[96, 220, 377, 457, 476, 481, 496]
$C_6H_{12}O_6$	L-sorbose (c)	−670.6	−303.6	[96, 476]
$C_6H_{12}O_6$	β-D-fructose (c)	−672.0	−302.2	[96, 144, 476]
$C_6H_{12}O_6$	D-mannose (c)	−672.3	−301.9	[496]
$C_6H_{14}O_6$	α-L-rhamnose monohydrate (c)	−711.2	−331.3	[476]
$C_6H_{14}O_7$	α-D-glucose hydrate (c)	−667.54	−374.97	[180, 181, 199, 529]
$C_7H_{14}O_6$	α-methyl-D-glucopyranoside (c)	−841.8	−294.8	[308, 442, 571]
$C_7H_{14}O_6$	β-methyl-D-glucopyranoside (c)	−840.8	−295.8	[442]
$C_7H_{14}O_6$	β-methyl-D-glucofuranoside (liq)	−849.1	−287.5	[442]
$C_7H_{14}O_7$	D-gluco-α-heptose (c)	−783.1	−353.5	[156]
$C_{12}H_{16}O_8$	levoglucosan triacetate (c)	−1303.8	−371.3	[220]
$C_{12}H_{18}O_8$	1,2-anhydroglucose-3,5,6-triacetate (c)	−1331.8	−411.7	[220]
$C_{14}H_{20}O_9$	rhamnose triacetate (c)	−1544.5	−455.4	[220]
$C_{16}H_{22}O_{11}$	glucose pentaacetate (c)	−1724.2	−532.1	[220]
$C_{16}H_{22}O_{11}$	galactose pentaacetate (c)	−1723.5	−532.8	[220]

α-D-xylose (c)—The combustion data of Skuratov, Strepikheev, and Kozina [442] were chosen in preference to the earlier work.

β-D- and B-L-arabinose (c)—The combustion data of Desai and Wilhoit [136] for D-arabinose (c) were used for the selection. Earlier combustion data refer

to L-arabinose but are much less precise.

β-D-ribose (c)—The combustion data of Desai and Wilhoit [136] were chosen in preference to the data of Stroh and Fincke [496].

levoglucosan (c)—The data of Skuratov, Strepikheev, and Kozina [442] were chosen in preference to other work.

β-L-rhamnose (c)—The data of Karrer and Fioroni [220] and Stohmann and Langbein [476] were averaged for the selection.

α-D-glucose (c)—The combustion data of Skuratov, Strepikheev and Kozina [442] and Huffman and Fox [199] were averaged to make the selection. The data on α-D-glucose prior to 1900 were not used.

α-D-glucose hydrate (c) *and β-D-glucose* (c)—The selected heats of combustion and heats of formation of β-D-glucose and α-D-glucose hydrate were obtained from the heat of solution data of Hendricks et al. [180, 181], Taylor and Rowlinson [529] and Sturtevant [498] on α-D-glucose, β-D-glucose and α-D-glucose hydrate in conjunction with the selected value for the heat of combustion of α-D-glucose (c).

α-D-galactose (c) — The combustion data of Stroh and Fincke [496] were chosen in preference to the earlier work, although the data of Karrer and Fioroni [220] and Stohmann and Langbein [476] are in good agreement with the selection. The combustion data of Clarke and Stegeman [96] appear not negative enough by 3 kcal mol⁻¹.

L-sorbose (c)—The data of Clarke and Stegeman [96] were chosen in preference to the data of Stohmann and Langbein [476].

β-D-fructose (c)—The combustion data of Clarke and Stegeman [96] were chosen in preference to the earlier work.

α-methyl-D-glucopyranoside (c)—The combustion data of Skuratov, Strepikheev, and Kozina [442] were chosen in preference to other work.

6.26. Disaccharides

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol⁻¹	$\Delta Hf°298$ K kcal mol⁻¹	Reference
$C_{12}H_{22}O_{11}$	sucrose (c)	−1348.2	−531.9	[76, 138, 152, 153, 162, 219, 220, 369, 377, 380, 381, 410, 420, 476, 481, 522, 540, 571]
$C_{12}H_{22}O_{11}$	β-lactose (c)	−1350.0	−530.1	[96, 162, 219, 220, 377, 457, 476, 481]
$C_{12}H_{22}O_{11}$	maltose (c)	−1349.3	−530.8	[219, 220, 230, 377, 476]
$C_{12}H_{22}O_{11}$	trehalose (c)	−1348.8	−531.3	[476]
$C_{12}H_{22}O_{11}$	cellobiose (c)	−1347.6	−532.5	[219, 220]
$C_{12}H_{24}O_{12}$	α-lactose monohydrate (c)	−1346	−602	[76, 96, 144, 162, 377, 457, 460, 476, 481]
$C_{12}H_{24}O_{12}$	β-maltose monohydrate (c)	−1342	−606	[96, 144, 377, 476]
$C_{12}H_{26}O_{13}$	trehalose dihydrate (c)	−1340.6	−676.1	[476]
$C_{20}H_{27}NO_{11}$	amygdalin (c)	−2348	−455	[35, 37]
$C_{28}H_{38}O_{19}$	sucrose octaacetate (c)	−3029.5	−901.9	[219, 220]
$C_{28}H_{38}O_{19}$	lactose octaacetate (c)	−3025.4	−906.0	[220]
$C_{28}H_{38}O_{19}$	maltose octaacetate (c)	−3026.9	−904.5	[219]
$C_{28}H_{38}O_{19}$	cellobiose octaacetate (c)	−3028.9	−902.5	[219, 220]

sucrose (c) — The combustion data of Verkade and Coops [540], and Dickinson [138] were chosen in preference to other work. The data of Rübner [410], Schläpfer and Fioroni [420], Wrede [571], Karrer and Fioroni [219, 220] and Ponomarev and Migarskaya [369] are in reasonable agreement with the selection.

β-lactose (c) — The combustion data of Karrer and Fioroni [219, 220] and Stohmann and Langbein [476] were averaged for the selection. The combustion data of Clarke and Stegeman [96] appears to be not negative enough by 4 kcal mol⁻¹.

maltose (c) — The data of Karrer and Fioroni [219, 220] and Stohmann and Langbein [476] were averaged for the selection.

α-lactose monohydrate (c) — The combustion data of Emery and Benedict [144], von Rechenberg [377], and Stohmann and Langbein [476] were averaged for the selection. The combustion data of Clarke and Stegeman [96] appear about 10 kcal mol⁻¹ too negative.

β-maltose monohydrate (c) — The combustion data of von Rechenberg [377] and Stohmann and Langbein [476] were averaged for the selection. The combustion data of Clarke and Stegeman [96] appear about 20 kcal mol⁻¹ too negative.

6.27. Oligosaccharides

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_{18}H_{32}O_{16}$	raffinose (c)	-2025	-761	[58, 457]
$C_{18}H_{32}O_{16}$	melezitose (c)	-1971	-815	[476]
$C_{18}H_{42}O_{21}$	raffinose pentahydrate (c)	-2066	-1122	[214, 215]
$C_{24}H_{40}O_{20}$	diamylose (c)	-2774	-850	[219, 418]
$C_{24}H_{42}O_{21}$	stachyose (c)	-2705	-987	[219]
$C_{36}H_{60}O_{30}$	α-tetramylose (c)	-4075	-1360	[219, 418]
$C_{48}H_{80}O_{40}$	β-hexamylose (c)	-5394	-1853	[219, 418]

Generally speaking, the combustion data on the oligosaccharides are very poor because of insufficient characterization of the samples and because of the lack of precision and accuracy found in the early combustion measurements. The overall uncertainty in the combustion data is 2 to 4 percent.

raffinose (c) — The bomb combustion data of Berthelot and Matignon [58] are preferred to the KClO$_3$ combustion data of Stohmann [457].

melezitose (c) — Stohmann and Langbein [476] gave the formula, $C_{18}H_{34}O_{17}$, which is that for the monohydrate, but called the compound anhydrous, giving a melting point of 157 °C. However, turanose, which is a hydrolysis product of melezitose, has a melting point of 157 °C. Pigman and Goepp [356] cite a melezitose dihydrate with a melting point of 153 to 154 °C. We have assumed the compound to be anhydrous in our calculations, using the formula, $C_{18}H_{32}O_{16}$.

6.28. Heterocyclic Oxygen Compounds

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_3H_4O_3$	ethylene carbonate (c)	-279.9	-138.9	[433]
C_3H_6O	oxacyclobutane (g) (trimethylene oxide).	-467.85	-19.25	[349]
C_4H_4O	furan (g)	-504.60	-8.23	[174, 358]
C_4H_4O	furan (liq)	-497.99	-14.84	[174, 246]
C_4H_8O	tetrahydrofuran (g)	-605.44	-44.03	[349]
C_4H_8O	tetrahydrofuran (liq)	-598.4	-51.1	[88, 442]
$C_4H_8O_2$	glycol acetal (liq)	-558.4	-91.1	[132]
$C_4H_8O_2$	1,3-dioxane (liq)	-559.48	-89.99	[155, 357, 445]
$C_4H_8O_2$	1,4-dioxane (liq)	-564.99	-84.47	[183, 405, 445]
$C_5H_4O_2$	furfural (liq)	-559.1	-47.8	[71, 94, 246, 312]
$C_5H_4O_3$	2-furoic acid (c) (pyromucic acid)	-487.8	-119.1	[71, 246, 318, 344, 460]
$C_5H_6O_2$	furfuryl alcohol (liq)	-609.2	-66.0	[246, 318, 344]
C_5H_8O	dihydropyran, 4H (liq)	-706.0	-37.5	[88]
$C_5H_{10}O$	tetrahydropyran (g)	-758.44	-53.39	[349]
$C_5H_{10}O$	tetrahydropyran (liq)	-750.7	-61.1	[88, 440, 442, 445]
$C_5H_{10}O_2$	tetrahydrofurfuryl alcohol (liq)	-707.7	-104.1	[246]
$C_6H_{10}O_4$	erythritol diformal (c)	-744.1	-161.8	[132]
$C_8H_{14}O_4$	erythritol diacetal (c)	-1049	-182	[132]
$C_9H_{14}O_6$	mannitol triformal (c)	-1083	-242	[132]
$C_{12}H_{20}O_6$	mannitol triacetal (c)	-1537	-275	[132]

furan (*liq*) — The combustion data of Guthrie et al. [174] were chosen in preference to the data of Landrieu et al. [246]. The unpublished data of Pilcher [358] on the heats of combustion and formation of furan (g) at 25 °C, $\Delta Hc° = -504.45 \pm 0.15$, and -8.39 ± 0.16 kcal mol^{-1}, are in excellent agreement with the value obtained by combining $\Delta Hc°$ (liq) with the heat of vaporization as determined by Guthrie et al. [174].

tetrahydrofuran (*liq*) — The combustion data of Skuratov, Strepikheev, and Kozina [442], and Cass, Fletcher, Mortimer, Springall, and White [88] were averaged in making the selection.

1,3-*dioxane and* 1,4-*dioxane* (*liq*) — The combustion data of Snelson and Skinner [445] were chosen in preference to other data.

furfural (*liq*) — Values of the heat of combustion ranged over three kilocalories per mole. No one piece of work seemed more accurate than another. The selection was made by averaging the data of Landrieu, Baylocq, and Johnson [246], Berthelot and Rivals [71], Chung-Cheng [94] and Miller [312].

2-furoic acid (*pyromucic acid*) (*c*) — The combustion

data of Parks, Mosley, and Peterson [344] were chosen in preference to other data.

furfuryl alcohol (*liq*) — The combustion data of Parks, Mosley and Peterson [344] were chosen in preference to other data.

tetrahydropyran (*liq*) — The combustion data of Skuratov, Strepikheev, and Kozina [442], and Snelson and Skinner [445] were averaged to make the selection.

6.29. Aliphatic Amines

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
CH_5N	methylamine (liq)	−253.5	−11.3	[206, 252, 520]
$CH_6N_2O_3$	methylamine nitrate (c)	−214.3	−84.7	[117, 304]
C_2H_7N	ethylamine (liq)	−409.5	−17.7	[206, 252, 520]
C_2H_7N	dimethylamine (liq)	−416.7	−10.5	[206, 252, 520]
$C_2H_8N_2$	ethylenediamine (liq)	−446.30	−15.06	[38, 166]
$C_2H_8N_2O_3$	ethylamine nitrate (c)	−373.7	−87.7	[117]
$C_2H_8N_2O_3$	dimethylamine nitrate (c)	−381.8	−79.6	[117]
$C_2H_{10}N_4O_6$	ethylenediamine dinitrate (c)	−373.5	−156.2	[302, 421]
C_3H_9N	n-propylamine (liq)	−565.31	−24.26	[252, 444, 520]
C_3H_9N	isopropylamine (liq)	−562.74	−26.83	[444]
C_3H_9N	trimethylamine (liq)	−578.6	−11.0	[206, 252, 520]
$C_3H_{10}N_2$	1,2-propanediamine (liq)	−600.35	−23.38	[166]
$C_3H_{10}N_2O_3$	trimethylamine nitrate (c)	−549.6	−74.1	[117]
$C_4H_{11}N$	n-butylamine (liq)	−721.42	−30.52	[145, 252, 520]
$C_4H_{11}N$	isobutylamine (liq)	−720.25	−31.68	[166, 252]
$C_4H_{11}N$	sec.-butylamine (liq)	−719.07	−32.87	[145, 252]
$C_4H_{11}N$	tert.-butylamine (liq)	−715.97	−35.97	[145, 252, 444, 520]
$C_4H_{11}N$	diethylamine (liq)	−727.2	−24.7	[206, 252, 323, 520]
$C_4H_{12}N_2$	1,2-butanediamine (liq)	−757.35	−28.74	[166]
$C_4H_{12}N_2$	2-methyl-1,2-propanediamine (liq)	−754.09	−32.00	[166]
$C_4H_{12}N_2O_3$	diethylamine nitrate (c)	−686.0	−100.1	[117]
$C_6H_{15}N$	triethylamine (liq)	−1044.6	−32.1	[206, 249, 252, 323, 520]
$C_6H_{16}N_2O_3$	triethylamine nitrate (c)	−1011.9	−98.9	[117]
$C_9H_{21}N$	tri-n-propylamine (liq)	−1515.26	−49.51	[249]

methylamine (*liq*) — The combustion data of Jaffe [206] were preferred to the earlier data.

methylamine nitrate (*c*) — The combustion data of Medard and Thomas [304] were preferred to those of Cottrell and Gill [117].

ethylamine (*liq*) — The combustion data of Jaffe [206] were preferred to the earlier data.

dimethylamine (*liq*) — The combustion data of Jaffe [206] were preferred to the earlier data.

ethylenediamine (*liq*) — The combustion data of Good and Moore [166] were preferred to those of Berthelot [38].

ethylenediamine dinitrate (*c*) — The combustion data of Medard and Thomas [302] were preferred to those of Schmidt [421].

n-propylamine (*liq*) — The combustion data of Smith and Good [444] were used to obtain the selected value.

trimethylamine (*liq*) — The combustion data of Jaffe

[206] were preferred to the earlier data.

n-butylamine (*liq*) — The combustion data of Evans, Fairbrother, and Skinner [145] were preferred to the earlier data.

isobutylamine (*liq*) — The combustion data of Good and Moore [166] were preferred to those of Lemoult [252].

sec.-butylamine (*liq*) — The combustion data of Evans, Fairbrother, and Skinner [145] were preferred to the earlier data.

tert.-butylamine (liq) — The combustion data of Evans, Fairbrother, and Skinner [145], and Smith and Good [444] were averaged to obtain the selected value.

diethylamine (liq) — The combustion data of Jaffe [206] were preferred to the earlier data.

triethylamine (liq) — The combustion data of Jaffe [206] were used to obtain the selected value. The combustion data of Lebedeva [249] ($\Delta Hc° = -1046.15$ kcal mol^{-1}, $\Delta Hf° = -30.54$ kcal mol^{-1}) are in reasonable agreement with the selection.

6.30. Aromatic Amines

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
C_6H_7N	aniline (liq)	−810.96	+7.55	[8, 104, 179, 195, 252, 353, 355, 460, 464, 465, 508, 509, 520, 551]
$C_6H_8N_2O_3$	aniline nitrate (c)	−793.9	−43.7	[117, 568]
C_7H_9N	N-methylaniline (liq)	−973.5	+7.7	[160, 354, 355, 551]
$C_8H_{11}N$	N,N-dimethylaniline (liq)	−1136.3	+8.2	[460, 551]

aniline (*liq*)—The combustion data of Hatton, Hildenbrand, Sinke, and Stull [179] were used to obtain the selected value. The combustion data of Anderson and Gilbert [8], Cole and Gilbert [104], and Huffman [195] are in good agreement with the selected value.

aniline nitrate (*c*)—The combustion data of Cottrell and Gill [117] were preferred to those of Willis [568].

N-methylaniline (*liq*)—The analysis of the thermodynamic data on aromatic amines by Vriens and Hill [551] was used in preference to the earlier combustion data.

N,N-dimethylaniline (*liq*)—The analysis of the thermodynamic data on aromatic amines by Vriens and Hill [551] was preferred to the early combustion data of Stohmann [460].

6.31. Aliphatic Amides

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
CH_3NO	formamide (liq)	−135.8	−60.7	[400, 489, 491]
$C_2H_3NO_3$	oxamic acid (c)	−130.2	−160.4	[293, 464, 465]
$C_2H_4N_2O_2$	oxamide (c)	−201.7	−123.0	[464, 465, 526]
C_2H_5NO	acetamide (c)	−282.9	−76.0	[51, 87, 489, 491]
$C_3H_6N_2O_2$	malonamide (c)	−356.6	−130.5	[464, 465, 524]
C_3H_7NO	propionamide (c)	−439.6	−81.7	[51, 489, 491]
C_3H_7NO	N,N-dimethylformamide (liq)	−464.1	−57.2	[308]
$C_3H_7NO_2$	ethylcarbamate (c) (urethane)	−396.9	−124.4	[464, 465]
$C_4H_7NO_2$	diacetamide (c)	−498	−117	[347]
$C_4H_8N_2O_2$	succinamide (c)	−510.6	−138.9	[464, 465, 526]
$C_4H_8N_2O_4$	L-tartramide (c)	−426.6	−222.9	[116, 526]
$C_4H_8N_2O_4$	meso-tartramide (c)	−426.0	−223.5	[116]
C_4H_9NO	n-butyramide (c)	−596.1	−87.5	[489, 491]

formamide (*liq*)—The combustion data of Roth and Banse [400] and Stohmann and Schmidt [489, 491] were used to obtain the selection.

oxamic acid (*c*)—The combustion data of Matignon [293], Stohmann [464], and Stohmann and Haussmann [465] were averaged to obtain the selection.

oxamide (*c*)—The combustion data of Tavernier and Lamouroux [526] were used to make the selection.

acetamide (*c*)—The data of Calvet [87] on the heat of solution of acetamide in NaOH(aq) were used in preference to the combustion data of Berthelot and Fogh [51] and Stohmann and Schmidt [489, 491].

malonamide (*c*)—The combustion data of Tavernier and Lamouroux [524] were used to make the selection.

propionamide (*c*)—The combustion data of Stohmann and Schmidt [489, 491] were preferred to those of Berthelot and Fogh [51].

succinamide (*c*)—The combustion data of Tavernier and Lamouroux [526] were preferred to the earlier work.

L-tartramide (*c*)—The combustion data of Coops and Verkade [116] were used in preference to that of Tavernier and Lamouroux [526]. The combustion data of Tavernier and Lamouroux [526] are less negative by 63 kcal mol^{-1}.

6.32. Aromatic Amides

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
C_7H_7NO	benzamide (c)	−849.04	−48.42	[8, 51, 104, 489, 491]
C_7H_7NO	formanilide (c)	−861.2	−36.2	[489, 491]
$C_8H_8N_2O_2$	phthalamide (c)	−921.3	−104.4	[464, 465]
C_8H_9NO	acetanilide (c)	−1009.5	−50.3	[51, 489, 491, 554]

6.32. Aromatic Amides—Continued

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_{10}H_{13}NO_2$	phenacetin (c)	-1283.5	-101.1	[251, 395]
$C_{13}H_{11}NO$	benzanilide (c)	-1576.1	-22.3	[51, 489, 491]

benzamide (c)—Cole and Gilbert [104] corrected the combustion data of Anderson and Gilbert [8]. The corrected data were the basis of our selected value.
acetanilide (c)—The data of Wadsö [554] on the heat of hydrolysis of acetanilide were used in preference to the early combustion data.

phenacetin (c)—The combustion data of Roth [395] were preferred to those of Lemoult [251].

benzanilide (c)—The combustion data of Stohmann and Schmidt [489, 491] were preferred to those of Berthelot and Fogh [51].

6.33. Urea, Guanidine, and Their Derivatives

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
CH_4N_2O	urea (c)	-150.97	-79.71	[67, 68, 144, 194, 242, 283, 410, 411, 457, 460, 475, 481]
CH_5N_3	guanidine (c)	-251.45	-13.39	[234]
$CH_5N_3O_4$	urea nitrate (c)	-130.0	-134.8	[302, 421]
$CH_5N_5O_2$	nitroaminoguanidine (c)	-270.13	$+5.29$	[301]
$CH_6N_4O_3$	guanidine nitrate (c)	-206.5	-92.5	[241, 292, 293]
$CH_8N_6O_3$	*sym*-diaminoguanidine nitrate (c)	-329.74	-37.57	[301]
$C_2H_4N_2O_2$	formylurea (c)	-207	-118	[289, 293]
$C_2H_4N_4O_2$	azodicarbamide (c)	-254.83	-69.90	[566]
$C_2H_5N_5O_3$	1-formamido-2-nitro-guanidine (c)	-323.8	-35.1	[566]
$C_2H_6N_4O_2$	hydrazodicarbamide (c)	-273.86	-119.19	[566]
$C_2H_7N_5O_4$	guanylurea nitrate (c)	-325.1	-102.1	[446]
$C_3H_6N_2O_3$	hydantoic acid (c) (ureido-acetic acid)	-308	-179	[307]
$C_3H_7N_5O_3$	1-acetamido-2-nitro-guanidine (c)	-475.0	-46.3	[566]
$C_3H_9N_5O_4$	acetamidoguanidine nitrate (c)	-471.5	-118.1	[566]
$C_3H_{12}N_6O_3$	guanidine carbonate (c)	-459.95	-232.10	[194, 306]
$C_4H_9N_3O_2$	creatine (c)	-555.46	-128.16	[144, 198, 475]
$C_4H_{11}N_3O_3$	creatine hydrate (c)	-552.8	-199.1	[475]

urea (c)—The combustion data of Huffman [194] and Månsson and Sunner [283] were averaged to make the selection.

urea nitrate (c)—The combustion data of Medard and Thomas [302] were used to make the selection.

guanidine nitrate (c)—The aqueous neutralization data of Krivtsov, Titova, and Rosolovskii [241] were used in

preference to the combustion data of Matignon [289, 293].

guanidine carbonate (c)—The combustion data of Huffman [194] were preferred to those of Medard and Thomas [306].

creatine (c)—The combustion data of Huffman, Ellis, and Fox [198] were chosen in preference to the earlier work.

6.34. Aliphatic Amino Acids

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_2H_5NO_2$	glycine (c)	-232.67	-126.22	[43, 144, 152, 200, 457, 475, 481, 535, 571]
$C_2H_6N_2O_5$	glycine nitrate (c)	-218.9	-174.1	[117]
$C_3H_7NO_2$	L-alanine (c)	-387.30	-133.96	[43, 144, 198, 535, 571]
$C_3H_7NO_2$	DL-alanine (c)	-386.71	-134.55	[148, 200, 460, 475, 571]
$C_3H_7NO_2$	sarcosine (c)	-400.1	-121.2	[85, 475]
$C_3H_7NO_2S$	L-cysteine (c)	-540.5	-124.6	[20, 81, 197, 501]

6.34. Aliphatic Amino Acids—Continued

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_3H_7NO_3$	L-isoserine (c)	−343.5	−177.8	[152, 571]
$C_3H_7NO_3$	L-serine (c)	−347.7	−173.6	[201]
$C_4H_7NO_4$	L-aspartic acid (c)	−382.84	−232.47	[43, 144, 152, 198, 331, 460, 475]
$C_4H_7NO_4$	diglycolamidic acid (c)	−395.8	−219.5	[462, 479]
$C_4H_8N_2O_3$	L-asparagine (c)	−460.97	−188.50	[43, 198, 457, 460, 475, 481]
$C_4H_9NO_2$	γ-aminobutyric acid (c)	−545.5	−138.1	[495]
$C_4H_9NO_3$	DL- and L-threonine (c)	−502.2	−181.4	[369, 535]
$C_4H_{10}N_2O_4$	L-asparagine monohydrate (c)	−458.26	−259.52	[144, 198]
$C_5H_9NO_2$	DL-proline (c)	−652.0	−125.7	[369]
$C_5H_9NO_3$	L-hydroxyproline (c)	−619.6	−158.1	[369]
$C_5H_9NO_4$	L-glutamic acid (c)	−536.2	−241.5	[144, 152, 198, 331, 536]
$C_5H_{10}N_2O_3$	L-glutamine (c)	−614.5	−197.3	[536]
$C_5H_{11}NO_2$	δ-aminovaleric acid (c)	−701.5	−144.5	[495]
$C_5H_{11}NO_2$	DL- and L-valine (c)	−697.8	−148.2	[439, 536, 571]
$C_5H_{11}NO_2S$	L-methionine (c)	−809.5	−180.4	[535]
$C_5H_{12}N_2O_2$	DL-ornithine (c)	−724.1	−156.0	[369]
$C_6H_9NO_6$	nitrilotriacetic acid (c)	−559.2	−312.5	[462, 479]
$C_6H_{12}N_2O_4S_2$	L-cystine (c)	−1016.3	−245.7	[20, 81, 144, 197, 501]
$C_6H_{13}NO_2$	α-aminocaproic acid (c) (norleucine)	−855.6	−152.7	[439, 495]
$C_6H_{13}NO_2$	γ-aminocaproic acid (c)	−853.9	−154.5	[495]
$C_6H_{13}NO_2$	δ-aminocaproic acid (c)	−854.6	−153.7	[495]
$C_6H_{13}NO_2$	e-aminocaproic acid (c)	−855.6	−152.7	[495]
$C_6H_{13}NO_2$	D-leucine (c)	−856.39	−151.97	[200]
$C_6H_{13}NO_2$	L-leucine (c)	−856.39	−151.97	[43, 152, 200, 460, 475, 536]
$C_6H_{13}NO_2$	DL-leucine (c)	−855.62	−152.74	[200]
$C_6H_{13}NO_2$	DL- and L-isoleucine (c)	−856.5	−151.8	[369, 535]
$C_6H_{14}N_2O_2$	DL-lysine (c)	−880.3	−162.2	[369]
$C_6H_{14}N_4O_2$	L-arginine (c)	−893.85	−148.66	[200]
$C_7H_{13}NO_3$	N-formyl-DL-leucine (c)	−880.3	−222.1	[571]
$C_7H_{15}NO_2$	ζ-aminoenanthylic acid (c)	−1011.1	−159.6	[495]
$C_9H_{19}NO_2$	ω-aminopelargonic acid (c)	−1321.4	−174.1	[495]
$C_{10}H_{16}N_2O_8$	ethylenediaminetetraacetic acid (c)	−1066.5	−420.5	[1]
$C_{12}H_{26}N_2O_4$	hexamethylene-1,6-diamine-adipic acid adduct (c)	−1711.2	−305.5	[495]
$C_{14}H_{23}N_3O_{10}$	diethylenetriamine-pentaacetic acid (c)	−1570.5	−531.8	[1]
$C_{14}H_{30}N_2O_4$	tetramethylene-1,4-diamine-sebacic acid adduct (c)	−2023.5	−317.9	[495]

glycine (*c*)—The data of Huffman, Fox, and Ellis [200] were chosen in preference to the other work. The data of Fischer and Wrede [152] and Emery and Benedict [144] are in good agreement with the selection.

L-alanine (*c*)—The data of Huffman, Ellis and Fox [198] were chosen in preference to earlier work. Although Huffman, Ellis, and Fox [198] designated their compound as *d*-alanine, examination of its configuration and specific rotation properties cited in Greenstein and Winitz [169] led us to feel the compound had the L-configuration.

DL-alanine (*c*)—The data of Huffman, Fox, and Ellis [200] were chosen in preference to the earlier work.

sarcosine (*c*)—The data of Breitenbach, Derkosch, and Wessely [85], and Stohmann, and Langbein [479] were averaged to make the selection.

L-cysteine (*c*)—The combustion data of Sunner [501] were chosen in preference to the earlier work. A correction was applied to bring the final state of sulfur in the combustion data to $H_2SO_4 \cdot 115H_2O(liq)$, and $\Delta Hf°[H_2SO_4 \cdot 115H_2O(liq)] = −212.192$ kcal mol^{-1}

L-serine (*c*)—Hutchens, Cole, and Stout [201] estimated the heat of formation to be −173.6 kcal mol^{-1}.

L-isoserine acid (*c*)—The work of Wrede [571] was used in making the selection.

L-aspartic acid (*c*)—The data of Huffman, Ellis, and Fox [198] were chosen in preference to those of other workers. Agreement with the data of Emery and Benedict [144] is good.

L-asparagine (*c*)—The data of Huffman, Ellis, and Fox [198] were chosen in preference to earlier work.

DL- and L-threonine (*c*)—The data of Ponomarev and

Migarskaya [369] were used for the selected value of both DL- and L-threonine. A value for $\Delta Hf°298$[L-threonine (c)] of -193.11 kcal mol^{-1} was calculated from the data of Tsuzuki, Harper, and Hunt [535], but was not used because of the poor agreement found between heats of formation reported for other amino acids by these authors and the values reported by other investigators. It was impossible to assign different values to DL and L isomers because of the lack of precise data on both compounds.

L-asparagine monohydrate (c)—The data of Huffman, Ellis, and Fox [198] were chosen in preference to the data of Emery and Benedict [144].

methionine (c)—The final state of sulfur in the combustion data was taken as $H_2SO_4 \cdot 115H_2O$(liq), and $\Delta Hf°[H_2SO_4 \cdot 115H_2O$(liq)] $= -212.192$ kcal mol^{-1}.

L-glutamic acid (c)—The data of Tsuzuki and Hunt [536] were chosen in preference to other work.

DL- and L-valine (c)—The data of Skuratov [439] and Tsuzuki and Hunt [536] both, on L-valine were averaged for the selected value for DL- and L-valine. The data of Wrede [571] on DL-valine are regarded as not accurate enough to assign a different value to these two forms.

L-cystine (c)—The combustion data of Sunner [501] were chosen in preference to the earlier work. The final state of sulfur in the combustion data was taken as $H_2SO_4 \cdot 115H_2O$(liq), and $\Delta Hf°[H_2SO_4 \cdot 115H_2O$ (liq)] $= -212.192$ kcal mol^{-1}.

L-leucine (c)—The data of Huffman, Fox, and Ellis [200] were chosen in preference to other work.

DL- and L-isoleucine (c)—The data of Ponomarev and Migarskaya [369] on DL-isoleucine were used for the selected value of both DL- and L-isoleucine. A value for $\Delta Hf°298$[L-isoleucine (c)] of -152.9 kcal mol^{-1} was calculated from the data of Tsuzuki, Harper, and Hunt [535], but was not used because of the poor agreement found between heats of formation reported for other amino acids by these authors and the values obtained by other investigators. It was impossible to assign different values to DL and L isomers because of the lack of precise data on both compounds.

L-arginine (c)—Although Huffman, Fox, and Ellis [200] designated their compound as *d*-arginine, examination of its configuration and specific rotation properties cited in Greenstein and Winitz [169] led us to feel the compound had the L-configuration.

6.35. Aromatic Amino Acids and Aliphatic Amino Acids Containing a Phenyl Group

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_7H_7NO_2$	o-aminobenzoic acid (c)	-801.7	-95.8	[250]
$C_7H_7NO_2$	m-aminobenzoic acid (c)	-799.3	-98.2	[250]
$C_7H_7NO_2$	p-aminobenzoic acid (c)	-798.7	-98.8	[250]
$C_8H_9NO_2$	N-phenyl glycine (c)	-963.6	-96.2	[152]
$C_8H_9NO_2$	α-phenyl glycine (c)	-956.6	-103.2	[152, 244]
$C_9H_9NO_3$	hippuric acid (c)	-1008.25	-145.63	[100, 104, 144, 148, 188, 193, 196, 450, 457, 460, 475, 481, 492, 557]
$C_9H_{11}NO_2$	DL- and L-phenylalanine (c)	-1110.3	-111.9	[85, 152, 535]
$C_9H_{11}NO_3$	L-tyrosine (c)	-1058.8	-163.4	[43, 144, 200, 331]
$C_{10}H_{11}NO_3$	phenaceturic acid (c)	-1165.2	-151.0	[490, 492]
$C_{10}H_{11}NO_3$	DL-benzoylalanine (c)	-1168.3	-147.9	[490, 492]
$C_{10}H_{11}NO_3$	benzoyl sarcosine (c)	-1180.5	-135.7	[490, 492]
$C_{10}H_{11}NO_3$	p-toluyl glycine (c)	-1167.7	-148.5	[490, 492]
$C_{10}H_{11}NO_3$	m-toluyl glycine (c)	-1167.4	-148.8	[490, 492]
$C_{10}H_{11}NO_3$	o-toluyl glycine (c)	-1167.9	-148.3	[490, 492]
$C_{10}H_{11}NO_4$	anisoyl glycine (c)	-1135.3	-180.9	[490, 492]
$C_{11}H_{12}N_2O_2$	L-tryptophane (c)	-1344.6	-99.8	[535]
$C_{11}H_{13}NO_3$	o-toluyl alanine (c)	-1322.1	-156.5	[490, 492]
$C_{11}H_{13}NO_3$	p-toluyl alanine (c)	-1319.6	-159.0	[490, 492]
$C_{12}H_{15}NO_4$	DL-phenylalanine-N-carboxylic acid dimethyl ester (c)	-1456.7	-184.3	[85]
$C_{16}H_{11}NO_2$	benzalhippuric acid azlactone (c)	-1850.0	-30.5	[152]
$C_{16}H_{13}NO_3$	benzalhippuric acid (c)	-1846.3	-102.6	[152]
$C_{16}H_{15}NO_3$	benzoylphenylalanine (c)	-1887.6	-129.6	[152]
$C_{17}H_{19}NO_2$	ethyl β-anilino-β-phenyl propionate (c)	-2165.1	-82.8	[370]
$C_{36}H_{44}N_2O_{10}$	L(+)-leucine methyl ester salt of (−)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3') (c)	-4358	-531	[243]
$C_{36}H_{44}N_2O_{10}$	L(+)-leucine methyl ester salt of (+)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3') (c)	-4349	-540	[243]

α-phenylglycine (c)—The combustion data of Fischer and Wrede [152], and Landrieu [244] were averaged to give the selected value.

hippuric acid (c)—The data of Hubbard, Frow and Waddington [188], Wagner [557], Fairbrother, Skinner, and Evans [148], Cole and Gilbert [104], and Huffman [193, 196] were averaged in making the selection. The data of Coates and Sutton [100] and Springhall, White

and Cass [450] were not used.

DL- and L-phenylalanine (c)—The data of Tsuzuki, Harper, and Hunt [535], Breitenbach, Derkosch, Wessely [85], and Fischer and Wrede [152] were averaged in making the selection. It was impossible to assign different values to the DL- and L-forms because of the lack of precise data on both compounds.

L-tyrosine (c)—The data of Huffman, Fox, and Ellis [200] were used in preference to other work.

6.36. Amino Acid Anhydrides
(Diketopiperazines)

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_4H_5NO_3$	sarcosine-N-carboxylic acid anhydride (c)	−402.9	−144.1	[85]
$C_4H_6N_2O_2$	glycine anhydride (c)	−475.1	−106.0	[152, 244, 571]
$C_6H_{10}N_2O_2$	alanine anhydride (c)	−777.9	−128.0	[152, 244, 300, 571]
$C_6H_{10}N_2O_4$	serine anhydride (c)	−696.4	−209.5	[368]
$C_7H_{12}N_2O_2$	glycylvalyl anhydride (c)	−947.7	−120.5	[585]
$C_8H_{14}N_2O_2$	valylalanyl anhydride (c)	−1107.3	−123.3	[368]
$C_{10}H_9NO_3$	phenylalanine-N-carboxylic acid anhydride (c)	−1115.6	−132.3	[85]
$C_{11}H_{12}N_2O_2$	glycylphenylalanyl anhydride (c)	−1361.6	−82.9	[368]
$C_{11}H_{12}N_2O_3$	glycyltyrosyl anhydride (c)	−1321.7	−122.8	[368]
$C_{11}H_{20}N_2O_2$	valylleucyl anhydride (c)	−1567.6	−150.1	[368]
$C_{12}H_{14}N_2O_2$	alanylphenylalanyl anhydride (c)	−1517.5	−89.3	[368]
$C_{12}H_{22}N_2O_2$	leucine anhydride (c)	−1720.1	−160.0	[152]
$C_{14}H_{18}N_2O_2$	valylphenylalanyl anhydride (c)	−1837.2	−94.3	[368]
$C_{18}H_{18}N_2O_2$	phenylalanyl anhydride (c)	−2238.5	−69.3	[585]

glycine anhydride (c)—The combustion data of Fischer and Wrede [152], Landrieu [244], and Wrede [571] were averaged to give the selected value.
alanine anhydride (c)—The combustion data of McEwan [300] were preferred to those of Fischer and

Wrede [152], Landrieu [244], and Wrede [571].

Sarcosine-N-carboxylic acid anhydride and phenyl-alanine-N-carboxylic acid anhydride are not diketo-piperazines.

6.37. Peptides

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_4H_8N_2O_3$	glycylglycine (c)	−470.95	−178.51	[152, 196, 244]
$C_5H_8N_2O_5$	glycylglycine-N-carboxylic acid (c)	−470.5	−273.0	[152, 571]
$C_5H_{10}N_2O_3$	DL-alanylglycine (c)	−626.19	−185.64	[196]
$C_6H_{11}N_3O_4$	diglycylglycine (c)	−709.2	−230.8	[571]
$C_6H_{12}N_2O_3$	ethyl glycylglycinate (c)	−803.7	−170.5	[152, 244]
$C_6H_{12}N_2O_5$	serylserine (c)	−692.4	−281.8	[367]
$C_7H_{14}N_2O_3$	glycylvaline (c)	−936.6	−200.0	[367]
$C_8H_{14}N_4O_5$	triglycylglycine (c)	−945.9	−284.7	[571]
$C_8H_{16}N_2O_3$	DL-leucylglycine (c)	−1093.86	−205.7	[196, 571]
$C_9H_{16}N_2O_5$	α-carbethoxyglycyl glycine ethyl ester (c)	−1117.7	−275.3	[152]
$C_9H_{16}N_2O_5$	β-carbethoxyglycylglycine ethyl ester (c)	−1089.5	−303.5	[152]
$C_{10}H_{19}N_3O_4$	leucylglycylglycine (c)	−1329.9	−259.6	[152]
$C_{11}H_{12}N_2O_4$	hippurylglycine (c)	−1245.92	−198.54	[196]
$C_{11}H_{14}N_2O_3$	glycylphenylalanine (c)	−1348.8	−163.9	[367]

6.37. Peptides—Continued

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta H f°298\ K$ kcal mol^{-1}	Reference
$C_{12}H_{16}N_2O_3$	alanylphenylalanine (c)	-1505.0	-170.2	[367]
$C_{14}H_{19}N_3O_4$	glycylalanylphenylalanine (c)	-1743.7	-222.0	[367]
$C_{14}H_{20}N_2O_3$	valylphenylalanine (c)	-1816.3	-183.5	[585]

glycylglycine (*c*)—The data of Huffman [196] were used in making the selection in preference to the earlier data.

glycylglycine-N-carboxylic acid (*c*)—The combustion data of Fischer and Wrede [152] and Wrede [571] were averaged to make the selection.

ethyl glycylglycinate (*c*)—The combustion data of Fischer and Wrede [152] and Landrieu [244] were averaged to give the selected value.

DL-leucylglycine (*c*)—The data of Huffman [196] were used in making the selection in preference to the data of Wrede [571].

6.38. Alkaloids

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_8H_{17}N$	coniine (liq)	-1275.5	-57.6	[35, 37]
$C_{17}H_{21}NO_4$	morphine monohydrate (c)	-2146.1	-170.1	[253, 256]
$C_{18}H_{23}NO_4$	codeine monohydrate (c)	-2327.3	-151.2	[254, 256]
$C_{19}H_{21}NO_3$	thebaine (c)	-2441.3	-63.0	[254, 256]
$C_{19}H_{22}N_2O$	cinchonidine (c)	-2545.5	$+7.1$	[52, 54]
$C_{19}H_{22}N_2O$	cinchonine (c)	-2545.8	$+7.4$	[52, 54]
$C_{19}H_{24}N_2O$	cinchonamine (c)	-2596.3	-10.4	[52, 54]
$C_{19}H_{25}N_3O_4$	cinchonamine nitrate (c)	-2561.0	-79.9	[52, 54]
$C_{20}H_{21}NO_4$	papaverine (c)	-2478.1	-120.2	[254, 256]
$C_{20}H_{24}N_2O_2$	quinidine (c)	-2662.5	-38.3	[52, 53]
$C_{20}H_{24}N_2O_2$	quinine (c)	-2663.7	-37.1	[52, 53]
$C_{21}H_{22}N_2O_2$	strychnine (c)	-2685.5	-41.0	[55, 56]
$C_{22}H_{23}NO_7$	narcotine (c)	-2643.8	-210.9	[254, 256]
$C_{23}H_{26}N_2O_4$	brucine (c)	-2932.7	-118.6	[55, 56]
$C_{23}H_{31}NO_{10}$	narceine dihydrate (c)	-2800.9	-421.2	[255, 256]

Cinchonine (c) and cinchonidine (c) are stereo-isomers, as are quinine (c) and quinidine (c). Differences in the values for their heats of combustion and formation should not be attributed to differences in configuration, but are more likely part of the experimental error in the measurements. Both references cited for each of the alkaloids refer to the same experimental data. Although the data are given to the nearest tenth of a kcal mol^{-1}, the uncertainties are more likely in the range 2 to 20 kcal mol^{-1}.

6.39. Heterocyclic Nitrogen Compounds

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
CH_2N_4	tetrazole (c)	-219.0	$+56.7$	[301]
CH_2N_4O	5-hydroxytetrazole (c)	-163.9	$+1.5$	[566]
CH_3N_5	5-aminotetrazole (c)	-246.2	$+49.7$	[301]
$CH_4N_6O_3$	5-aminotetrazole nitrate (c)	-224.1	-6.6	[301]
C_2HN_5	5-cyanotetrazole (c)	-318.3	$+96.1$	[566]
$C_2H_2N_6$	3-azido-s-triazole (c)	-361.9	$+105.5$	[135]
$C_2H_3N_7$	4-amino-3-azido-s-triazole (c)	-427.1	$+136.5$	[135]
$C_2H_4N_4$	3-amino-1,2,4-triazole (c)	-343.1	$+18.4$	[566]
$C_2H_4N_4O$	5-methoxytetrazole (c)	-341.3	$+16.6$	[566]
$C_2H_4N_{10}$	5,5'-hydrazotetrazole (c)	-459.8	$+135.1$	[301]
C_2H_5N	ethylenimine (liq)	-380.86	$+21.97$	[324]
$C_2H_5N_5$	1-methyl-5-aminotetrazole (c)	-405.14	$+46.25$	[565, 566]
$C_2H_5N_5$	2-methyl-5-aminotetrazole (c)	-409.3	$+50.4$	[565, 566]
$C_2H_5N_5$	5-methylaminotetrazole (c)	-407.2	$+48.4$	[566]
$C_2H_5N_7$	5-guanylaminotetrazole (c)	-399.4	$+40.5$	[301]
$C_2H_5N_5O_3$	3-amino-1,2,4-triazole nitrate (c)	-318.0	-40.9	[566]

6.39.   Heterocyclic Nitrogen Compounds — Continued

Formula	Compound (State)	$\Delta Hc°298\ K$ kcal mol^{-1}	$\Delta Hf°298\ K$ kcal mol^{-1}	Reference
$C_2H_8N_{10}O$	1-(5-tetrazolyl)-4-guanyltetra- zene monohydrate (c)	−506.5	+45.2	[566]
$C_3H_2N_2O_3$	parabanic acid (c)	−212.5	−138.0	[290, 293]
$C_3H_4N_2$	imidazole (c)	−433.3	+14.5	[24]
$C_3H_4N_2$	pyrazole (c)	−447.1	+28.3	[24]
$C_3H_4N_2O_2$	hydantoin (c)	−311.6	−107.2	[307]
$C_3H_4N_6$	3-azido-5-methyl-s-triazole (c)	−512.6	+93.8	[135]
$C_3H_5N_5O$	5-acetamidotetrazole (c)	−451.7	−1.2	[301]
$C_3H_5N_7$	4-amino-3-azido-5-methyl-s- triazole (c)	−568.6	+115.6	[135]
$C_3H_6N_4$	1,5-dimethyl tetrazole (c)	−532.2	+45.1	[301]
$C_3H_6N_4O$	1,4-dimethyl-5-tetrazolone (c)	−480.5	−6.6	[566]
$C_3H_6N_6$	melamine (c)	−469.8	−17.3	[413, 414, 525]
$C_3H_7N_5$	5-dimethylaminotetrazole (c)	−564.9	+43.6	[566]
$C_3H_7N_5O_3$	3-amino-5-methyl-1,2,4- triazole nitrate (c)	−466.7	−54.6	[566]
$C_3H_8N_6O_3$	1,3-dimethyl-5-imino- tetrazole nitrate (c)	−554.1	−1.3	[566]
$C_4H_4N_2$	pyrazine (g)	−559.69	+46.86	[533]
$C_4H_4N_2$	pyrazine (c)	−546.24	+33.41	[533]
$C_4H_4N_2$	pyridazine (g)	−579.35	+66.52	[533]
$C_4H_4N_2$	pyridazine (liq)	−566.57	+53.74	[533]
$C_4H_4N_2$	pyrimidine (g)	−559.82	+46.99	[533]
$C_4H_4N_2$	pyrimidine (liq)	−547.87	+35.04	[533]
$C_4H_4N_2O_3$	barbituric acid (c)	−360.6	−152.2	[152, 294]
$C_4H_4N_2O_4$	dialuric acid (c)	−198.4	−314.4	[294]
$C_4H_4N_2O_5$	alloxan monohydrate (c)	−273.76	−239.08	[288, 294, 456]
C_4H_5N	pyrrole (g)	−572.87	+25.88	[424]
C_4H_5N	pyrrole (liq)	−562.07	+15.08	[45, 424]
$C_4H_5N_3O_3$	uramil (c) (5-aminobarbituric acid)	−378.8	−168.2	[294]
$C_4H_6N_2O_2$	5-methyl hydantoin (c)	−464.8	−116.3	[524]
$C_4H_6N_4O_3$	allantoin (c)	−409.64	−171.51	[144, 288, 293, 456]
$C_4H_6N_6$	3-azido-5-ethyl-s-triazole (c)	−668.5	+87.4	[135]
$C_4H_6N_8$	1,2-di-(5-tetrazolyl)ethane (c)	−687.3	+106.2	[566]
$C_4H_6N_{10}$	cis-1,1′-dimethyl-5,5′-azotet- razole (c)	−769.7	+188.6	[566]
$C_4H_6N_{10}$	trans-1,1′-dimethyl-5,5′-azotet- razole (c)	−770.5	+189.3	[566]
$C_4H_6N_{10}$	2,2′-dimethyl-5,5′-azotetra- zole (c)	−761.5	+180.3	[566]
C_4H_7NO	α-pyrrolidone (c)	−547.0	−68.3	[494]
$C_4H_7N_3O$	creatinine (c)	−558.54	−56.77	[144, 198]
$C_4H_7N_5$	1-allyl-5-aminotetrazole (c)	−678.7	+63.4	[566]
$C_4H_7N_5$	2-allyl-5-aminotetrazole (c)	−682.9	+67.6	[566]
$C_4H_7N_7$	4-amino-3-azido-5-ethyl-s- triazole (c)	−733.8	+118.5	[135]
$C_4H_7N_5O_2$	5-tetrazolylurethan (c)	−562.7	−52.6	[301]
C_4H_9N	pyrrolidine (g)	−682.73	−0.89	[296]
C_4H_9N	pyrrolidine (liq)	−673.75	−9.87	[185, 296]
$C_4H_{10}N_2$	piperazine (c)	−706.88	−10.90	[23]
$C_4H_{22}N_2O_6$	piperazine hexahydrate (c)	−690.9	−436.8	[36, 38]
$C_5H_4N_4O$	hypoxanthine (c) (6-oxypurine)	−580.65	−26.24	[39, 40, 456]
$C_5H_4N_4O$	8-oxypurine (c)	−591.4	−15.4	[39, 40]
$C_5H_4N_4O_2$	xanthine (c)	−516.39	−90.49	[45, 46, 456]
$C_5H_4N_4O_3$	isouric acid (c)	−459.0	−147.9	[294]
$C_5H_4N_4O_3$	uric acid (c)	−459.16	−147.73	[144, 287, 294, 456, 457, 460, 475, 481]
C_5H_5N	pyridine (g)	−674.65	+33.61	[121, 188]

6.39. Heterocyclic Nitrogen Compounds—Continued

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
C_5H_5N	pyridine (liq)	−665.00	+23.96	[111, 121, 130, 131, 188, 493, 512]
C_5H_5NO	pyrrolaldehyde (c)	−616.3	−24.8	[453]
$C_5H_5N_5$	adenine (c)	−664.25	+23.21	[456]
$C_5H_5N_5O$	guanine (c)	−597.33	−43.72	[456, 475]
$C_5H_6N_2O$	pyrrolaldoxime (c)	−678.9	+3.7	[453]
$C_5H_6N_2O_2$	4-methyluracil (c)	−566.0	−109.2	[152]
$C_5H_6N_2O_2$	thymine (c) (5-methyl uracil)	−563.3	−111.9	[152]
$C_5H_6N_2O_3$	dimethyl parabanic acid (c)	−538.2	−137.0	[291, 293]
$C_5H_6N_4O_4$	pseudouric acid (c)	−453.5	−221.7	[294]
$C_5H_7N_3$	2,6-diaminopyridine (c)	−707.9	−1.5	[143, 572]
$C_5H_8N_2O_2$	5,5-dimethyl hydantoin (c)	−617.1	−126.4	[300, 524]
$C_5H_8N_2O_2$	4-methylhydrouracil (c)	−618.0	−125.5	[152]
$C_5H_8N_4O_3$	methyl allantoin (c) (pyvurile)	−566.6	−177.0	[293]
C_5H_9N	1,2,5,6-tetrahydropyridine (liq)	−785.7	+8.0	[23]
C_5H_9NO	α-piperidone (c)	−704.4	−73.3	[494]
C_5H_9NO	N-methylpyrrolidone (liq)	−715.03	−62.64	[240]
$C_5H_{11}N$	piperidine (liq)	−824.94	−21.05	[23, 130, 131]
$C_6H_4N_2$	3-cyanopyridine (c)	−747.17	+46.23	[413, 414]
$C_6H_5NO_2$	picolinic acid (c)	−651.4	−83.7	[579]
$C_6H_5N_3$	benzotriazole (c)	−794.84	+59.74	[147]
$C_6H_6N_4$	7-methylpurine (c)	−820.6	+51.3	[39, 40]
$C_6H_6N_4O$	7-methylhypoxanthine (c)	−759.4	−9.9	[39, 40]
C_6H_7N	2-methylpyridine (g)	−827.46	+24.05	[121, 426]
C_6H_7N	2-methylpyridine (liq)	−817.24	+13.83	[111, 121, 408, 426]
C_6H_7N	3-methylpyridine (g)	−829.71	+26.30	[121, 425]
C_6H_7N	3-methylpyridine (liq)	−818.98	+15.57	[111, 121, 408, 425]
C_6H_7N	4-methylpyridine (g)	−827.85	+24.44	[121]
C_6H_7N	4-methylpyridine (liq)	−816.99	+13.58	[111, 121, 408]
$C_6H_{10}N_2O_2$	5-methyl-5-ethyl hydantoin (c)	−770.9	−135.0	[524]
$C_6H_{10}N_{10}$	2,2'-diethyl-5,5'-azotetrazole (c)	−1062.5	+156.6	[566]
$C_6H_{11}NO$	e-caprolactam (c)	−861.4	−78.6	[494]
$C_6H_{11}NO$	N-methyl piperidone (liq)	−870.04	−70.00	[240]
$C_6H_{12}N_2$	triethylenediamine (c)	−970.8	−3.4	[346]
$C_6H_{12}N_4$	hexamethylenetetramine (c)	−1002.9	+28.7	[14, 15, 125, 127, 133]
$C_6H_{14}N_6O_6$	hexamethylenetetramine dinitrate (c)	−953.9	−88.6	[125, 127, 133]
$C_7H_6N_4$	1-phenyltetrazole (c)	−949.8	+86.5	[301]
$C_7H_6N_4$	5-phenyltetrazole (c)	−933.3	+70.0	[301]
$C_7H_6N_4O$	1-phenyl-5-hydroxytetrazole (c)	−890.0	+26.7	[301]
C_7H_7N	2-vinylpyridine (liq)	−934.7	+37.2	[18]
$C_7H_7N_5$	1-phenyl-5-aminotetrazole (c)	−971.8	+74.3	[566]
$C_7H_7N_5$	5-phenylaminotetrazole (c)	−970.4	+72.9	[566]
$C_7H_8N_4O_2$	theobromine (c)	−845.2	−86.4	[291, 294]
C_7H_9N	2-ethylpyridine (liq)	−964.6	−1.2	[18]
C_7H_9N	2,3-dimethylpyridine (liq)	−970.40	+4.62	[122]
C_7H_9N	2,4-dimethylpyridine (liq)	−969.63	+3.85	[122]
C_7H_9N	2,5-dimethylpyridine (liq)	−970.23	+4.45	[121, 122]
C_7H_9N	2,6-dimethylpyridine (liq)	−968.80	+3.02	[111, 121, 122]
C_7H_9N	3,4-dimethylpyridine (liq)	−970.14	+4.36	[122]
C_7H_9N	3,5-dimethylpyridine (liq)	−971.14	+5.36	[122]

6.39. Heterocyclic Nitrogen Compounds—Continued

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_7H_{11}N_5$	1-allyl-5-allylaminotetrazole (c)	−1117.8	+83.7	[566]
$C_7H_{11}N_5$	5-diallylaminotetrazole (c)	−1118.0	+83.9	[566]
$C_7H_{13}NO$	N-methylcaprolactam (liq)	−1029.1	−73.3	[240]
$C_7H_{13}NO$	5-methylcaprolactam (c)	−1015.5	−86.9	[494]
$C_7H_{13}NO$	7-methylcaprolactam (c)	−1015.9	−86.5	[494]
$C_7H_{13}NO$	ζ-enantholactam (c)	−1019.2	−83.2	[494]
$C_8H_5NO_2$	isatin (c)	−860.5	−62.7	[5, 453]
$C_8H_6N_4O_6$	hydurilic acid (c)	−658.2	−299.2	[294]
$C_8H_6N_6$	3-azido-5-phenyl-s-triazole (c)	−1084.5	+127.1	[135]
C_8H_7N	indole (c)	−1021.3	+29.8	[45, 46, 452]
C_8H_7NO	oxindole (c)	−950.3	−41.2	[45, 46]
$C_8H_7NO_2$	dioxindole (c)	−914.6	−76.9	[5]
$C_8H_7N_7$	4-amino-3-azido-5-phenyl-s-triazole (c)	−1151.0	+159.5	[135]
$C_8H_8N_4$	1-methyl-5-phenyltetrazole (c)	−1095.6	+69.9	[566]
$C_8H_8N_4$	1-phenyl-5-methyltetrazole (c)	−1095.6	+69.9	[301, 566]
$C_8H_8N_4$	2-phenyl-5-methyltetrazole (c)	−1091.3	+65.7	[301]
$C_8H_8N_6O_6$	murexide (c)	−736.0	−289.7	[294]
$C_8H_{10}N_4O_2$	caffeine (c) (methyl theobromine)	−1017.8	−76.2	[291, 294, 475]
$C_8H_{10}N_4O_{10}$	alloxantin dihydrate (c)	−583.7	−510.3	[288, 294]
$C_8H_{12}N_2O_3$	diethylbarbituric acid (c) (veronal)	−983.6	−178.7	[152]
C_9H_7N	quinoline (liq)	−1122.9	+37.3	[128, 131]
C_9H_7N	isoquinoline (c)	−1123.5	+37.9	[129, 313]
C_9H_7NO	8-hydroxyquinoline (c)	−1065.7	−19.9	[499, 500, 570]
$C_9H_8N_2O$	di-α-pyrrylketone (c)	−1115.0	−4.7	[452]
C_9H_9N	α-methylindole (c)	−1168.4	+14.5	[45, 46]
C_9H_9N	skatole (c)	−1170.2	+16.3	[45, 46]
$C_9H_{10}N_2$	dipyrrylmethane (c)	−1219.4	+31.4	[452]
$C_9H_{15}N$	phyllopyrrole (c) (2,4,5-trimethyl-3-ethyl pyrrole)	−1338.4	−20.4	[453]
$C_{10}H_8N_2O_2$	4-phenyl uracil (c)	−1132.1	−81.7	[152]
$C_{10}H_9N$	N-phenylpyrrole (c)	−1286.0	+38.1	[452, 462]
$C_{10}H_9N$	α-phenylpyrrole (c)	−1282.4	+34.5	[452]
$C_{10}H_9N$	quinaldine (c) (α-methyl quinoline)	−1287.2	+39.3	[128, 131]
$C_{10}H_{14}N_2$	nicotine (liq)	−1428.1	+9.4	[45, 46]
$C_{12}H_8N_2$	phenazine (c)	−1458.3	+56.4	[6, 568]
$C_{12}H_9N$	carbazole (c)	−1466.3	+30.3	[45, 46, 526]
$C_{12}H_{14}N_4O_6$	desoxyamalic acid (c)	−1321.1	−285.7	[294]
$C_{12}H_{14}N_4O_8$	amalic acid (c)	−1239.8	−367.0	[294]
$C_{13}H_9N$	acridine (c)	−1574.9	+44.8	[6, 568]
$C_{16}H_{10}N_2O_2$	indigotin (c)	−1814	−32	[5]
$C_{16}H_{12}N_2O_4$	isatide (c)	−1776	−139	[5]
$C_{21}H_{16}N_2$	lophine (c)	−2587	+65	[131]
$C_{21}H_{18}N_2$	amarine (c)	−2653	+63	[126, 131]
$C_{21}H_{19}N_2O_{0.5}$	amarine hemihydrate (c)	−2653	+29	[126, 131]
$C_{24}H_{24}N_2O_3$	anisine (c)	−3026	−51	[126, 131]

melamine (c) — The combustion data of Salley and Gray [413, 414] and Tavernier and Lamouroux [525] were averaged to make the selection.

pyrrole (liq) — The combustion data of Scott et al. [424] were used for the selection in preference to the earlier work of Berthelot and Andre [45].

barbituric acid (c) — The combustion data of Fischer and Wrede [152] were selected in preference to the work of Matignon [294].

alloxan monohydrate (c) — The combustion data of Stieh-

ler and Huffman [456] were chosen in preference to the earlier work of Matignon, [288, 294].

allantoin (*c*) — The combustion data of Stiehler and Huffman [456] were chosen in preference to the earlier work for the selected value.

creatinine (*c*) — The combustion data of Huffman, Ellis, and Fox [198] were chosen in preference to the data of Emery and Benedict [144].

pyrrolidine (*liq*) — The combustion data of McCullough et al. [296] were chosen for the selection. The value obtained by Hildenbrand et al. [185], for the enthalpy of combustion of pyrrolidine is in excellent agreement with the selection.

hypoxanthine (*c*) — The combustion data of Stiehler and Huffman [456] were chosen in preference to the data of Berthelot [39, 40].

xanthine (*c*) — The combustion data of Stiehler and Huffman [456] were chosen in preference to the data of Berthelot and Andre [45, 46].

uric acid (*c*) — The combustion data of Stiehler and Huffman [456] were chosen in preference to the earlier work.

guanine (*c*) — The combustion data of Stiehler and Huffman [456] were chosen in preference to the data of Stohmann and Langbein [475].

pyridine (*g*) — The heat of vaporization of pyridine is an average value obtained from the data of Cox et al. [121], and Hubbard et al. [188]; the heat of vaporization of pyridine was taken to be 9.65 kcal mol⁻¹. This value was then combined with the combustion data on pyridine (liq).

pyridine (*liq*) — The combustion data of Cox, Challoner, and Meetham [121], and Hubbard, Frow, and Waddington [188] were averaged to make the selection. The early work of Delepine [130, 131] is in good agreement with the selection by about 0.1 kcal mol⁻¹; this is perhaps fortuitous. The remaining combustion data [111, 493, 512] vary between 7 and 14 kcal mol⁻¹ from the selected value.

5,5-dimethylhydantoin (*c*) — The combustion data of Tavernier and Lamouroux [524] and McEwan [300] were averaged to make the selection.

piperidine (*liq*) — The combustion data of Bedford, Beezer, and Mortimer [23] were chosen for the selected value. The data of McCullough and co-workers, $\Delta Hc°$ [piperidine (liq)] at 25 °C = − 825.29 ± 0.11 kcal mol⁻¹, cited in reference [23] are in good agreement with the selected value. We have not used the data of McCullough and co-workers because their work has not yet appeared as a formal publication. The data of Delepine

[130, 131] were not used.

2-methylpyridine (*g*) *and* (*liq*) — The combustion data of Scott et al. [426], and Cox, Challoner, and Meetham [121] were averaged in making the selection. Similar treatment was given to the data [121, 188] on the heat of vaporization as for pyridine. The data of Constam and White [111], and Roth and Müller [408] were not used.

3-methylpyridine (*g*) *and* (*liq*) — The combustion data of Scott et al. [425], and Cox, Challoner, and Meetham [121] were used in making the selection. Similar treatment was given to the data [121, 188] on the heat of vaporization as with pyridine. The data of Constam and White [111], and Roth and Müller [408] were not used.

4-methylpyridine (*liq*) — The combustion data of Cox, Challoner, and Meetham [121] were used in making the selection in preference to the earlier data of Constam and White [111], and Roth and Müller [408].

hexamethylenetetramine (*c*) — The combustion data of Delepine and Badoche [133] were used for the selected value in preference to their earlier work.

hexamethylenetetramine dinitrate (*c*) — The combustion data of Delepine and Badoche [133] were used in preference to the earlier work of Delepine [125, 127].

2,5-dimethylpyridine (*liq*) — The combustion data of Cox and Gundry [122] were used in preference to the earlier work of Cox, Challoner, and Meetham [121].

2,6-dimethylpyridine (*liq*) — The combustion data of Cox and Gundry [122] were used in preference to the earlier work of Cox, Challoner, and Meetham [121] and Constam and White [111].

isatin (*c*) — The combustion data of Stern and Klebs [453] were used in preference to the data of d'Aladern [5].

indole (*c*) — The combustion data of Stern and Klebs [452], and Berthelot and Andre [45, 46] were averaged to make the selection.

1-phenyl-5-methyltetrazole (*c*) — The combustion data of McEwan and Riggs [301] and Williams, McEwan and Henry [566] were averaged to make the selection.

caffeine (*c*) — The combustion data of Matignon [291, 294] and Stohmann and Langbein [475] were averaged to make the selection.

8-hydroxyquinoline (*c*) — The combustion data of Sullivan [499], Sullivan and Hunt [500] and Wood and Jones [570] were averaged to obtain the selected value.

carbazole (*c*) — The combustion data of Tavernier and Lamouroux [526] were used in making the selection in preference to the data of Berthelot and Andre [45, 46].

6.40. Porphyrins

Formula	Compound (State)	$\Delta Hc°$298 K kcal mol⁻¹	$\Delta Hf°$298 K kcal mol⁻¹	Reference
$C_{32}H_{36}N_4O_2$	pyrroporphyrin (XV) mono-methyl ester (c)	− 4150.7	− 88.6	[454]
$C_{32}H_{38}N_4$	aetioporphyrin (I)(c)	− 4305.8	− 1.8	[454]
$C_{32}H_{38}N_4$	aetioporphyrin (II)(c)	− 4312.0	+ 4.4	[454]
$C_{33}H_{38}N_4O_2$	γ-phylloporphyrin mono-methyl ester (c)	− 4314.4	− 87.3	[454]
$C_{34}H_{34}N_4O_4$	protoporphyrin (c)	− 4238.5	− 120.6	[454]
$C_{34}H_{36}N_4O_3$	phylloerythrin monomethyl ester (c)	− 4344.2	− 83.2	[454]
$C_{34}H_{36}N_4O_3$	pyropheophorbide *a* mono-methyl ester (c)	− 4342.6	− 84.8	[454]

6.40. Porphyrins—Continued

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_{34}H_{36}N_4O_4$	verdoporphyrin dimethyl ester (c)	-4284.1	-143.3	[454]
$C_{34}H_{36}N_4O_5$	pheopurpurin 18 monomethyl ester (c)	-4196.6	-230.8	[454]
$C_{34}H_{38}N_4O_2$	desoxyphylloerythrin monomethyl ester (c)	-4456.8	-38.9	[454]
$C_{34}H_{38}N_4O_4$	rhodoporphyrin (XV) dimethyl ester (c)	-4373.5	-122.2	[454]
$C_{34}H_{38}N_4O_4$	rhodoporphyrin (XXI) dimethyl ester (c)	-4371.8	-123.9	[454]
$C_{35}H_{38}N_4O_5$	chloroporphyrin e_5 dimethyl ester (c)	-4486.5	-103.3	[454]
$C_{35}H_{40}N_4O_4$	chlorin e_4 dimethyl ester (c)	-4513.2	-144.9	[454]
$C_{35}H_{40}N_4O_4$	chloroporphyrin e_4 dimethyl ester (c)	-4503.9	-154.2	[454]
$C_{36}H_{36}N_4O_6$	methyl pheophorbide b (c)	-4414.8	-200.7	[454]
$C_{36}H_{38}N_4O_4$	protoporphyrin dimethyl ester (c)	-4561.7	-122.1	[454]
$C_{36}H_{38}N_4O_5$	methyl pheophorbide a (c)	-4527.7	-156.1	[454]
$C_{36}H_{38}N_4O_5$	phcoporphyrin a_5 dimethyl ester (c)	-4519.5	-164.3	[454]
$C_{36}H_{40}N_4O_6$	chlorin p_6 trimethyl ester (c)	-4460.1	-292.0	[454]
$C_{36}H_{42}N_4O_4$	mesoporphyrin (IX) dimethyl ester (c)	-4624.1	-196.4	[454]
$C_{36}H_{46}N_4$	octaethyl porphyrin (c)	-4917.2	$-39.9.$	[454]
$C_{37}H_{40}N_4O_7$	dimethyl pheopurpurin 7 (c)	-4600.4	-245.8	[454]
$C_{37}H_{42}N_4O_6$	chloroporphyrin e_6 trimethyl ester (c)	-4684.2	-230.3	[454]
$C_{37}H_{42}N_4O_6$	chlorin e_6 trimethyl ester (c)	-4693.1	-221.4	[454]
$C_{40}H_{46}N_4O_8$	coproporphyrin (I) tetramethyl ester (c)	-4985.0	-348.3	[454]
$C_{48}H_{54}N_4O_{16}$	iso-uroporphyrin (II) octamethyl ester (c)	-5738.9	-620.1	[454]

Although the data on the porphyrins are given to the nearest tenth of a kcal mol^{-1}, the uncertainties are more likely in the range 2 to 20 kcal mol^{-1}.

6.41. Organic Sulfur Compounds

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
CH_4S	methanethiol (liq)	-363.48	-11.08	[165]
C_2H_4S	thiacyclopropane (liq)	-481.02	$+12.41$	[502, 505]
C_2H_6S	ethanethiol (liq)	-519.39	-17.53	[41, 298]
C_2H_6S	2-thiapropane (liq)	-521.37	-15.55	[298]
$C_2H_6S_2$	1,2-ethanedithiol (liq)	-667.97	-12.83	[282]
$C_2H_6S_2$	2,3-dithiabutane (liq)	-665.98	-14.82	[157, 187]
C_3H_6S	thiacyclobutane (liq)	-636.90	$+5.93$	[190, 295, 502, 505]
C_3H_8S	1-propanethiol (liq)	-675.51	-23.78	[192]
$C_3H_8S_2$	1,3-propanedithiol (liq)	-824.34	-18.83	[282]
C_4H_4S	thiophene (liq)	-675.95	$+19.24$	[157, 191, 295, 317, 504, 505, 553]
C_4H_8S	thiacyclopentane (liq)	-775.95	-17.39	[124, 190, 295, 502, 505]

6.41. Organic Sulfur Compounds—Continued

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
$C_4H_{10}S$	1-butanethiol (liq)	−831.97	−29.69	[189]
$C_4H_{10}S_2$	1,4-butanedithiol (liq)	−980.42	−25.11	[282]
C_5H_6S	2-methylthiophene (liq)	−829.83	+10.75	[350]
C_5H_6S	3-methylthiophene (liq)	−829.46	+10.38	[299]
$C_5H_{10}S$	thiacyclohexane (liq)	−930.38	−25.33	[295, 297, 502, 505]
$C_5H_{12}S$	1-pentanethiol (liq)	−988.30	−35.72	[41,190, 295, 503, 505]
C_6H_6S	benzenethiol (liq)	−928.45	+15.32	[427]
$C_6H_{14}S$	1-hexanethiol (liq)	−1144.55	−41.84	[163]
C_7H_8S	benzyl mercaptan (liq)	−1086.0	+10.4	[272, 275]
C_7H_8S	phenyl methyl sulfide (liq)	−1087.0	+11.5	[272, 273]
$C_{12}H_{10}S$	diphenyl sulfide (c)	−1653.2	+39.1	[272, 274]
$C_{12}H_{10}S_2$	diphenyl disulfide (c)	−1793.7	+35.8	[272, 274]

We have used $H_2SO_4 \cdot 115H_2O$ (liq) as the final state of sulfur in the combustion values cited above, and have taken $\Delta Hf°[H_2SO_4 \cdot 115H_2O(\text{liq})] = -212.192$ kcal mol^{-1} at 298.15 K.

ethanethiol (liq)—The combustion data of McCullough et al. [298] were preferred to the earlier data of Berthelot [41].

2,3-dithiabutane (liq)—The combustion data of Hubbard et al. [187] were preferred to those of Franklin and Lumpkin [157].

thiacyclobutane (liq)—The combustion data of Hubbard, Katz, and Waddington [190] and Sunner [505] were averaged to obtain the selected value.

thiophene (liq)—The combustion data of Hubbard,

Scott, Frow and Waddington [191], and Sunner [505] were averaged to obtain the selected value.

thiacyclopentane (liq)—The combustion data of Hubbard, Katz, and Waddington [190], and Sunner [505] were averaged to obtain the selected value.

thiacyclohexane (liq)—The combustion data of McCullough et al. [297] and Sunner [505] were averaged to obtain the selected value.

1-pentanethiol (liq)—The combustion data of Sunner [505] were chosen in preference to those of Hubbard, Katz, and Waddington [190] because they were in better agreement with the energy term for the CH_2 increment in the liquid state.

6.42. Organic Sulfur Compounds Containing Nitrogen and/or Oxygen

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
CH_4N_2S	thiourea (c)	−353.43	−21.13	[20, 293, 504]
C_2H_4OS	thiolacetic acid (liq)	−416.22	−52.39	[504, 505]
$C_2H_7NO_3S$	2-aminoethane-1-sulfonic acid (c) (taurine)	−383.4	−187.7	[34]
$C_3H_4N_2OS$	thiohydantoin (c)	−503.2	−59.5	[294]
$C_3H_6O_2S$	β-thiolactic acid (liq)	−519.4	−111.6	[81, 197]
$C_3H_6N_2O_2S$	thiohydantoic acid (c)	−498.4	−132.6	[294]
$C_3H_7NO_2S$	L-cysteine (c)	−540.5	−124.6	[20, 81, 197, 501]
$C_4H_2N_2S$	4-cyanothiazole (c)	−641.03	+52.63	[284]
C_4H_5NS	4-methylthiazole (liq)	−707.18	+16.31	[284]
$C_5H_{11}NO_2S$	L-methionine (c)	−809.5	−180.4	[535]
$C_6H_{10}O_4S_2$	β,β'-dithiodilactic acid (liq)	−962.7	−230.9	[81, 197]
$C_6H_{12}N_2S_3$	tetramethylthiuram monosulfide (c)	−1417.43	+11.60	[164]
$C_6H_{12}N_2S_4$	tetramethylthiuram disulfide(c)	−1559.64	+9.94	[164]
$C_6H_{12}N_2O_4S_2$	L-cystine (c)	−1016.3	−245.7	[20, 81, 144, 197, 501]

We have used $H_2SO_4 \cdot 115H_2O(\text{liq})$ as the final state for the sulfur in the combustion values cited above, and have taken $\Delta Hf,[H_2SO_4 \cdot 115H_2O(\text{liq})] = -212.192$ kcal mol^{-1} at 298.15 K.

thiourea (c)—The combustion data of Sunner [504]

were preferred to any earlier data.

L-cysteine (c)—The combustion data of Sunner [501] were chosen in preference to the earlier work.

L-cystine (c)—The combustion data of Sunner [501] were chosen in preference to the earlier work.

6.43. Organic Phosphorus Compounds

Formula	Compound (State)	$\Delta Hc°298$ K kcal mol^{-1}	$\Delta Hf°298$ K kcal mol^{-1}	Reference
C_3H_9P	trimethylphosphine (liq)	−763	−30	[258]
$C_6H_{15}O_4P$	triethyl phosphate (liq)	−983	−297	[25, 328]
$C_9H_{21}O_4P$	tri-n-propyl phosphate (liq)	−1452	−315	[415]
$C_{12}H_{27}OP$	tri-n-butyl phosphine oxide (c)	−2143	−110	[451]
$C_{12}H_{27}O_2P$	n-butyl ester of di-n-butyl-phosphinic acid (liq)	−2071	−183	[451]
$C_{12}H_{27}O_4P$	tri-n-butyl phosphate (liq)	−1906 (−1921)	−348 (−333)	[328, 451]
$C_{12}H_{27}O_4P$	triisobutyl phosphate (liq)	−1908	−346	[328]
$C_{18}H_{15}O_4P$	triphenyl phosphate (c)	−2228	−181	[328]

The combustion data on organic phosphorus compounds are, in general, very poor. None of the measurements were made in a rotating-bomb calorimeter, which would insure homogeneity of the phosphoric acid solution formed during the combustion. Appropriate data to provide the information needed for the reduction of the bomb process to standard conditions are not available. Most of the combustion data are uncertain by 0.25 to 0.5 percent. We have adjusted the combustion data so that $H_3PO_4(c)$ appears as the final standard state of phosphorus, and have used $\Delta Hf°[H_3PO_4(c)] = −305.7$ kcal mol^{-1}. Both references cited for tri-n-butyl phosphate (liq) refer to the same experimental data. The values in parentheses are calculated from the data on tri-n-propyl phosphate and the CH_2(liq) increment.

triethyl phosphate (liq) — The combustion data of Bedford and Mortimer [25] were preferred to those of Nikolaev, Afanas'ev, and Starostin [328].

7. References

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8. Compound Index

A

*(WLN denotes the Wiswesser Line Notation. For further information, the reader should see: Smith, E. G., The Wiswesser Line-Formula Chemical Notation (McGraw-Hill Book Company, 1968; Library of Congress Card Number 68–13107).)

Compound name, page	Empirical formula, WLN

Compound name, page	Empirical formula, WLN

Compound name, page	Empirical formula, WLN

Compound name, page   Empirical formula, WLN

Q

Compound name, page

R

Empirical formula, WLN

raffinose, 244

$C_{18}H_{32}O_{16}$, T6OTJ B1Q CQ DQ EQ FO1- BT6OTJ CQ DQ
EQ FO- BT5OTJ B1Q CQ DQ E1Q -A&BCD -B&EF
-A&BD -B&CEF -A&D -B&BCE

raffinose pentahydrate, 244

$C_{18}H_{42}O_{21}$, T6OTJ B1Q CQ DQ EQ FO1- BT6OTJ CQ DQ
EQ FO- BT5OTJ B1Q CQ DQ E1Q -A&BCD -B&EF
-A&BD -B&CEF -A&D -B&BCE &/QH 5

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rhamnose triacetate, 242
rhodoporphyrin (XV) dimethyl ester, 256

$C_6H_6O_2$, QR CQ
$C_6H_{12}O_5$, T6OTJ BQ CQ DQ EQ F -A&BCDF -B&E
$C_6H_{14}O_6$, T6OTJ BQ CQ DQ EQ F -A&CDF -B&BE &QH
$C_{14}H_{20}O_9$, T6OTJ BQ COV1 DOV1 EOV1 F -A&CDF -B&E
$C_{34}H_{38}N_4O_4$, T D5 I5 N5-16-5 A D- I- N- AM D-N
I-M N-NJ EVO1 F J2 K O2 P T U2VO1

rhodoporphyrin (XXI) dimethyl ester, 256

$C_{34}H_{38}N_4O_4$, T D5 I5 N5-16-5 A D- I- N- AM D-N
I-M N-NJ EVO1 F J K2VO1 O P2 T2 U

β-D-ribose, 242
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rye bread, 277

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serine anhydride, 250
serylserine, 250
skatole, 254
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$C_7H_6O_2$, VHR BQ
$C_7H_6O_3$, QVR BQ
$C_3H_7NO_2$, QV1M1
$C_4H_5NO_3$, T5NVOV EHJ A

$C_3H_7NO_3$, QVYZ1Q -B
$C_6H_{10}N_2O_4$, T6MV DM EVTJ C1Q F1Q
$C_6H_{12}N_2O_5$, QVYY1QMVYZ1Q
C_9H_9N, T56 BMJ D
$C_6H_8O_2$, QV1U2U2
$C_6H_{12}O_6$, Q1YQYQYQV1Q -ABA
$C_{24}H_{42}O_{21}$, T6OTJ B1Q CQ DQ EQ/ FO1- BT6OTJ CQ DQ
EQ/ 2 FO- BT5OTJ B1Q CQ DQ E1Q/ -A&BCD
-B&EF/ 2 -A&BD -B&CEF -A&D -B&BCE

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starch hexaacetate, 277

$C_{18}H_{36}O_2$, QV17

strychnine, 251

$C_{21}H_{22}N_2O_2$, T6 G656 B7 C6 E5 D 5ABCEF A& FX MNV
QO VN SU AHT&&TTTTJ

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$C_4H_6O_4$, QV2VQ
$C_4H_4O_3$, T5VOVTJ
$C_{12}H_{22}O_{11}$, T6OTJ B1Q CQ DQ EQ FO- BT5OTJ B1Q CQ
DQ E1Q -A&BD -B&CEF -A&BD -B&CE

sucrose octaacetate, 243

$C_{28}H_{38}O_{19}$, T6OTJ B1OV1 COV1 DOV1 EOV1 FQ- BT5OTJ
B1OV1 COV1 DOV1 E1OV1 -A&BD -B&CEF -A&BD
-B&CE

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$C_4H_6O_6$, QVYQYQVQ
$C_4H_8O_7$, QVYQYQVQ &QH
$C_4H_6O_6$, QVYQYQVQ -AB
$C_4H_8N_2O_4$, ZVYQYQVZ -AB

$C_7H_{10}O_4$, T5OVTJ DVQ E E

$C_7H_{10}O_4$, QV1YVQUY

C_4H_8O, T5OTJ
$C_5H_{10}O_2$, T5OTJ B1Q
$C_5H_{10}O$, T6OTJ
C_5H_9N, T6M CUTJ
$C_{14}H_{30}N_2O_4$, QV6VQ &Z4Z
$C_6H_{12}N_2S_4$, 1N1&YUS&S 2
$C_6H_{12}N_2S_3$, 1N1&YUS& 2S
$C_{36}H_{60}O_{30}$, T6OTJ BQ CQ DQ F1Q EO-/ BT6OTJ CQ DQ
F1Q EO-/ 4 BT6OTJ CQ DQ EQ F1Q / -A&BCE
-B&DF/ 6

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CH_2N_4, T5MNNNJ
$C_2H_8N_{10}O$, T5MNNNJ ENUNMMYZUM &QH
$C_4H_7N_5O_2$, T5MNNNJ EMVO2
$C_{19}H_{21}NO_3$, T B6566 B6/CO 4ABBC R BX HO PN
GH&&TTJ FO1 JO1 P
$C_7H_8N_4O_2$, T56 BN DN FNVMVJ B F
C_3H_6S, T4STJ
$C_5H_{10}S$, T6STJ

9. Miscellaneous Comments

We wish to call attention to several publications which have been found during the course of preparing this manuscript which seem of value for one reason or another.

First, U.S. Department of Agriculture Handbook No. 74 (Merrill and Watt [588]) contains an accurate evaluation of the energy values of foods associated with problems of nutrition. Combustion data on a large number of specific protein, fat, and carbohydrate substances are reported. Relationships between metabolism, digestibility, and the available energy of foods are also given.

Second, we call attention to some combustion studies on a group of substances which are not part of our main listing of compounds, but are of biological interest. They have been excluded from our listing because they (1) are not well characterized, (2) are polymeric, (3) contain elements other than CHNOPS, or (4) had combustion measurements made upon them which were not very precise. These combustion data are useful only in the sense that they provide a rough estimate of the heats of combustion of the respective substances. The references and substances are given below.

Stohmann, von Rechenberg, Wilsing and Rodatz [481], and Stohmann [457]
    cellulose
    inulin
    potato starch
    rice starch
    linseed oil
    olive oil
    poppy seed oil
    seed extracts
    butter
    human fat
    animal fat
    blood fibrin
    egg albumin
    milk casein

    paraglobulin
    conglutin
    rye bread
    wheat bread

Stohmann [463]
    dextran
    inulin
    starch
    cellulose

Karrer and Fioroni [219, 220]
    xylan
    diacetyl xylan
    starch hexaacetate
    cellulose hexaacetate
    inulin hexaacetate

Emery and Benedict [144]
    glycogen

Collatz [107]
    calcium 1-glycerol phosphate
    calcium hexose diphosphate

Clarke and Datta [98]
    dipotassium glucose-1-phosphate
    disodium glycerol-1-phosphate
    disodium glycerol-2-phosphate

Tsuzuki, Harper, and Hunt [535]
    insulin

Ponomarev [365]
    wheat grain protein
    (gluten, gliadin, glutenin)

Breitenbach, Derkosch, and Wessely [85]
    phenylalanine polypeptide
    sarcosine polypeptide