

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 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.

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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 semi-quantitative 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, ΔH_c° , 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, ΔH_f° , are expressed in kcal mol⁻¹ (column 4), and were calculated by combining the appropriate data for the heats of formation of CO₂(g), H₂O(l), H₃PO₄(c), and H₂SO₄ · 115H₂O(l) 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

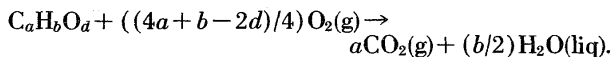
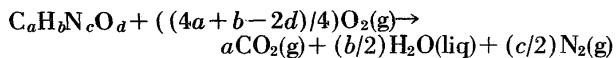
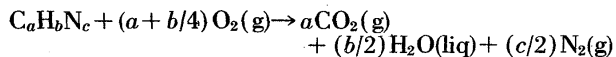
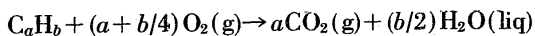
¹ Figures in brackets indicate literature references (Section 7).

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 investigations and (5) exposition of random and

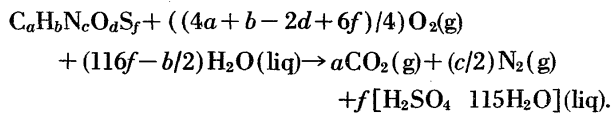
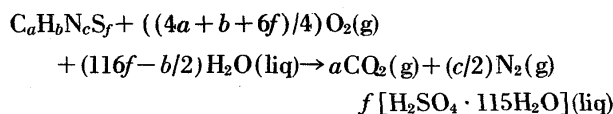
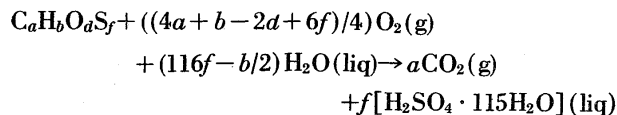
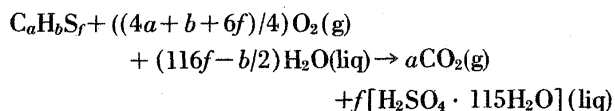
systematic errors. cursory presentation of data, or lack of adequate discussion, often leaves persistent doubts as to the quality of the study. A well-documented presentation answers questions about the sample, the procedures, or the treatment of the results which most thermochemists would raise.

3. Generalized Combustion Reactions for CHNOPS Compounds

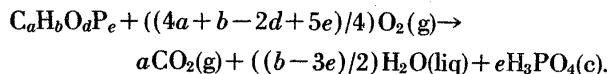
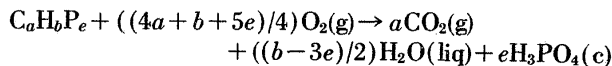
In order to calculate the heats of formation of organic compounds of the type: C_aH_b , $C_aH_bN_c$, $C_aH_bN_cO_d$, or $C_aH_bO_d$ from their corresponding heats of combustion, only the heats of formation of $CO_2(g)$ and $H_2O(lig)$ are needed. Organic nitrogen compounds form $N_2(g)$ as a product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



To calculate the heats of formation of 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 $CO_2(g)$, $H_2O(lig)$ and $H_2SO_4 \cdot 115H_2O(lig)$ are needed. Care must be taken to account for the $((b/2) - f)H_2O(lig)$ formed as a product in these combustions, which is not written as a discrete product, but becomes incorporated into the aqueous sulfuric acid solution.



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 $CO_2(g)$, $H_2O(lig)$, and $H_3PO_4(c)$ are required.



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 "Thermochemische 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 $\text{H}_2\text{SO}_4 \cdot 115\text{H}_2\text{O}$ (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 $^\circ$.

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, $-\Delta U_B = 26434 \pm 3 \text{ Jg}^{-1}$ (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 $\text{C}^{12} = 12$ [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 ΔC_p 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 ΔH_f° 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), $-94.051 \text{ kcal mol}^{-1}$; water (liq), $-68.315 \text{ kcal mol}^{-1}$; phosphoric acid (c), $-305.7 \text{ kcal mol}^{-1}$; and aqueous sulfuric acid, $\text{H}_2\text{SO}_4 \cdot 115\text{H}_2\text{O}$, $-212.192 \text{ kcal mol}^{-1}$. 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 $8.3143 \text{ J deg}^{-1} \text{ mol}^{-1}$. 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 ΔH_c° or ΔH_f° is cited to: (kcal mol^{-1})	The estimated uncertainty in ΔH_c° or ΔH_f° 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

The program under which this work was performed was initiated at the National Bureau of Standards on 1 May 1964 and has continued up to the present time. The substances included were selected for their relevance to biologically related problems. The thermodynamic data are to be used by NASA in studying problems such as: (1) theoretically recovering part of the pre-biological history of the earth, (2) examining the occurrence of organic compounds naturally synthesized under primitive conditions, and (3) inferring as much as possible of the thermodynamics and thermochemistry of inaccessible environments from a limited amount of information. Technical supervision was provided by Dr. George Jacobs of the National Aeronautics and Space Administration, Dr. Charles W. Beckett and Dr. George T. Armstrong, both of the National Bureau of Standards. We also acknowledge the valuable consultative assistance of Dr. Harold Morowitz, Department of Molecular Biology and Biophysics, Yale University. The work at NBS for NASA is coordinated with a related task at the Thermodynamics Research Center, Texas A&M University, under the supervision of Dr. Randolph C. Wilhoit, and a more comprehensive compilation of the thermodynamic data prepared will appear in "Handbook of Thermodynamic Data for Biochemistry" (Academic Press, Inc.), G. T. Armstrong and R. C. Wilhoit, editors.

The author acknowledges the important role of (Mrs.) Iva Halow Day in the present work. Her efforts in collection, evaluation, and selection of a large segment of the combustion and formation data presented here are greatly appreciated. The author also thanks his wife, Carol, for her assistance in compiling the references, and Mr. William J. Wiswesser for proofreading the Wiswesser Line-Formula Notations cited in the compound index.

6. Classes of Compounds and Selected Values

6.1. Aliphatic Hydrocarbons

Formula	Compound (State)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
CH ₄	methane (g)	-212.79	-17.89	[10, 32, 150, 315, 387, 388, 530, 531, 578]
C ₂ H ₂	acetylene (g)	-310.61	+54.19	[31, 32, 62, 315, 316, 531, 556, 578, 590,]
C ₂ H ₄	ethylene (g)	-337.23	+12.50	[10, 32, 62, 141, 150, 168, 235, 315, 316, 375, 391, 531, 578]
C ₂ H ₆	ethane (g)	-372.81	-20.24	[62, 390, 531, 578]
C ₃ H ₈	propane (g)	-530.57	-24.84	[62, 390, 531, 578]
C ₄ H ₁₀	<i>n</i> -butane (g)	-687.68	-30.10	[390, 578, 589]
C ₅ H ₁₂	<i>n</i> -pentane (g)	-845.16	-34.99	[359, 390, 578]
C ₅ H ₁₂	<i>n</i> -pentane (liq)	-838.78	-41.37	[404, 373, 578, 584]
C ₆ H ₁₄	<i>n</i> -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], Mixer [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 Mixer [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 Mixer [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 Zubo [576] as corrected by Swietoslawski [516] are of historical interest only.

6.2. Alicyclic Hydrocarbons

Formula	Compound (State)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₃ H ₆	cyclopropane (g)	-499.85	+12.75	[32, 62, 63, 238, 578]
C ₄ H ₈	cyclobutane (liq)	-650.22	+0.76	[113, 217, 578]
C ₅ H ₁₀	cyclopentane (liq)	-786.55	-25.28	[113, 213, 448, 516, 577, 578]
C ₆ H 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ 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 $\Delta H_c^\circ[\text{C}_6\text{H}_6(\text{liq})] = -780.96$ kcal mol⁻¹, we calculate $\Delta H_c^\circ = -789.06$ 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, Dieneske, 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, $\Delta H_c^\circ[\text{C}_{10}\text{H}_8(\text{c})] = -1231.8$ kcal mol⁻¹, we calculate $\Delta H_c^\circ = -1249.4$ 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], Rüber 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 ($-\Delta U_B = 26434$ Jg⁻¹ (vacuum) at 25 °C), and apply the appropriate corrections (for standard states, ΔnRT , and calculation of ΔH_f°), we obtain for our selected values $\Delta H_c^\circ = -1231.8$ kcal mol⁻¹, and $\Delta H_f^\circ = +18.0$ 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 $\Delta H_c^\circ[\text{C}_{14}\text{H}_{10}(\text{c})] = -1687.3$ kcal mol⁻¹, we calculate $\Delta H_c^\circ = -1712.0$ 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. $\Delta H_c^\circ[\text{C}_{14}\text{H}_{10}(\text{c})] = -1687.3$ 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 $\Delta H_c^\circ[\text{C}_{14}\text{H}_{10}(\text{c})] = -1685.6$ kcal mol⁻¹, we calculate $\Delta H_c^\circ = -1706.7$ 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 Vieille [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. $\Delta H_c^\circ[\text{C}_{14}\text{H}_{10}(\text{c})] = -1685.6$ 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ 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 CH₃OH(liq) is obtained by combining the value for the heat of combustion of CH₃OH(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], ΔH_{vap} 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 ΔH_{vap} at 25 °C = 9.08 kcal mol⁻¹ for the process: CH₃OH(liq) = CH₃OH(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 Ranse [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 CH₃CH₂OH(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], ΔH_{vap} 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: CH₃CH₂OH(liq) = CH₃CH₂OH (g, monomer), ΔH_{vap} 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₆ H ₆ O	phenol (c)	-729.80	-39.45	[9, 16, 57, 75, 118, 119, 218, 280, 341, 377, 457, 460, 476, 484]
C ₆ H ₆ O ₂	pyrocatechol (c)	-683.0	-86.3	[457, 460, 476]
C ₆ H ₆ O ₂	resorcinol (c)	-681.30	-87.95	[137, 457, 460]
C ₆ H ₆ O ₂	hydroquinone (c)	-681.78	-87.47	[29, 57, 277, 280, 341, 363, 460, 476, 484, 523, 537]
C ₇ H ₈ O	<i>o</i> -cresol (c)	-882.72	-48.90	[9, 118, 119, 485]
C ₇ H ₈ O	<i>m</i> -cresol (c)	-885.25	-46.37	[9, 118, 119, 485, 510, 511]
C ₇ H ₈ O	<i>p</i> -cresol (c)	-883.99	-47.63	[9, 118, 119, 485]
C ₈ H ₁₀ O	2-ethylphenol (c)	-1044.07	-49.91	[77]
C ₈ H ₁₀ O	3-ethylphenol (c)	-1042.77	-51.21	[77]
C ₈ H 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₂ H ₆ O ₂	1,2-ethanediol (liq) (ethylene glycol)	-284.35	-108.70	[216, 260, 322, 345, 476]
C ₃ H ₈ O ₂	1,2-propanediol (liq)	-435.8	-119.6	[259, 322]
C ₃ H ₈ O ₂	1,3-propanediol (liq)	-431.0	-124.4	[259]
C ₃ H ₈ O ₃	1,2,3-propanetriol (liq) (glycerol)	-395.65	-159.76	[144, 260, 345, 457, 481]
C ₄ H ₁₀ O ₄	meso-1,2,3,4-butanetetrol (c) (meso-erythritol)	-500.22	-217.56	[58, 270, 345, 457, 460, 476]
C ₅ H ₁₂ O ₄	pentaerythritol (c)	-660.1	-220.0	[305, 476]
C ₅ H ₁₂ O ₅	xylitol (c)	-612.83	-267.32	[330]
C ₅ H ₁₂ O ₅	L-arabitol (c)	-611.4	-268.7	[476]
C ₆ H ₁₂ O ₃	acetone glycerol (liq)	-811	-163	[17]
C ₆ H ₁₄ O ₆	D-mannitol (c)	-722.97	-319.54	[17, 76, 162, 345, 377, 457, 476, 481]
C ₆ H ₁₄ O ₆	dulcitol (c)	-720.68	-321.83	[76, 345, 377, 457, 476, 481]
C ₇ H ₁₆ O ₇	D-perseitol (c)	-835.2	-369.7	[476]
C ₇ H ₁₆ O ₇	D-glucio- 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 Louguine [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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₂ H ₆ O	dimethyl ether (g)	-349.06	-43.99	[32, 360, 531]
C ₃ H ₈ O	methyl ethyl ether (g)	-503.69	-51.72	[360, 531]
C ₄ H ₁₀ O	diethyl ether (g)	-657.52	-60.26	[361, 458, 531]
C ₄ H 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
CH ₂ O	formaldehyde (g) (methanal)	-136.42	-25.95	[558, 591]
C ₂ H ₂ O ₂	glyoxal (g)	-205.76	-50.66	[591]
C ₂ H ₄ O	acetaldehyde (g) (ethanal)	-285.01	-39.72	[65, 139]
C ₂ H ₄ O	acetaldehyde (liq) (ethanal)	-278.77	-45.96	[49, 50, 105, 406]
C ₃ H ₆ O	<i>n</i> -propionaldehyde (liq) (1-propanal)	-434.1	-53.0	[49, 50, 534]
C ₃ H ₆ O ₃	glyceraldehyde (liq)	-344	-143	[17]
C ₄ H ₈ O	<i>n</i> -butyraldehyde (liq) (1-butanal)	-592.2	-57.3	[326, 534]
C ₅ H ₁₀ O	<i>n</i> -valeraldehyde (liq) (1-pentanal)	-742	-70	[262]
C ₅ H ₁₀ O ₂	5-hydroxy-1-pentanal (liq)	-697.1	-114.7	[442]
C ₆ H ₁₀ O ₃	acetone glyceraldehyde (liq)	-726	-180	[17]
C ₆ H ₁₂ O ₃	paraldehyde (liq)	-810.0	-164.2	[90, 155, 265]
C ₇ H ₆ O	benzaldehyde (liq)	-843.2	-20.1	[246, 487]
C ₇ H ₆ O ₂	salicylaldehyde (liq)	-796.4	-66.9	[71, 134, 386]
C ₇ H ₁₄ O	<i>n</i> -heptaldehyde (liq)	-1062.2	-74.4	[261, 326]
C ₈ H ₁₆ O	<i>n</i> -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 ΔH_c° 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₃ H ₆ O	propanone (g) (acetone)	-435.32	-51.78	[310, 531]
C ₃ H ₆ O	propanone (liq) (acetone)	-427.92	-59.18	[49, 50, 144, 351, 528]
C ₄ H ₈ O	butanone (g) (methyl ethyl ketone)	-590.20	-59.26	[123]
C ₄ H ₈ O	butanone (liq) (methyl ethyl ketone)	-584.17	-65.29	[317, 344, 378, 436, 516]

6.9. Ketones—Continued

Formula	Compound (State)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₄ H ₆ O ₂	2,3-butanedione (liq) (diacetyl)	-493.71	-87.44	[245, 327, 341, 449]
C ₅ H ₁₀ O	2-pentanone (liq) (methyl <i>n</i> -propyl ketone)	-740.78	-71.05	[178, 516, 575]
C ₅ H ₁₀ O	3-pentanone (liq) (diethyl ketone)	-740.96	-70.87	[178, 264, 406, 516, 575]
C ₈ H ₈ O	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], $\Delta H_{\text{vap}}^\circ$ 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
CH ₂ O ₂	formic acid (liq) (methanoic acid)	-60.86	-101.51	[34, 59, 60, 208, 248, 434]
C ₂ H ₄ O ₂	acetic acid (liq) (ethanoic acid)	-209.02	-115.71	[59, 60, 146, 248, 395, 416, 417]
C ₃ H ₆ O ₂	propionic acid (liq) (propanoic acid)	-365.03	-122.07	[248, 265, 417, 472, 473]
C ₄ H ₈ O ₂	butyric acid (liq) (butanoic acid)	-521.87	-127.59	[248, 472, 473]
C ₅ H ₁₀ O ₂	valeric acid (liq) (pentanoic acid)	-678.12	-133.71	[3, 176, 248, 472, 473]
C ₆ H ₁₂ O ₂	caproic acid (liq) (hexanoic acid)	-834.49	-139.71	[3, 152, 248, 263]
C ₇ H ₁₄ O ₂	enanthic acid (liq) (heptanoic acid)	-990.81	-145.75	[3, 248]
C ₈ H ₁₆ O ₂	caprylic acid (liq) (octanoic acid)	-1147.00	-151.93	[3, 248, 266, 267]
C ₉ H 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ 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 Schj  nberg [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, $\Delta H(\text{fusion})$ 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₂ H ₄ O ₃	glycolic acid (c) (hydroxyacetic acid)	-166.1	-158.6	[271, 460]
C ₂ H ₄ O ₄	glyoxylic acid (c)	-125.0	-199.7	[34, 61]
C ₃ H ₄ O ₃	pyruvic acid (c)	-278.5	-140.3	[79]
C ₃ H ₄ O ₆	mesoxalic acid (c)	-128.1	-290.7	[294]
C ₃ H ₆ O ₃	D-lactic acid (c)	-321.22	-165.88	[415]
C ₃ H ₆ O ₃	DL-lactic acid (liq)	-326.8	-160.3	[144, 271]
C ₄ H ₈ O ₃	DL- β -hydroxybutyric acid (liq)	-487.2	-162.3	[144]
C ₄ H ₈ O ₃	hydroxyisobutyric acid (c)	-471.6	-177.9	[269, 271]
C ₅ H ₈ O ₃	levulinic acid (c) (γ -ketovaleric acid)	-576.9	-166.6	[44]
C ₆ H ₁₂ O ₇	D-galactonic acid (c)	589.4	-384.8	[497]
C ₆ H 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₃ H ₄ O ₂	acrylic acid (liq)	-327.0	-91.8	[321, 385]
C ₄ H ₆ O ₂	<i>cis</i> -crotonic acid (liq)	-498	-83	[99]
C ₄ H ₆ O ₂	<i>trans</i> -crotonic acid (c)	-478.2	-102.9	[462]
C ₅ H ₈ O ₂	angelic acid (c) (<i>trans</i> - α,β - dimethylacrylic acid)	-634.6	-108.9	[461, 462]
C ₅ H ₈ O ₂	tiglic acid (c) (<i>cis</i> - α,β - dimethylacrylic acid)	-626.2	-117.3	[461, 462]
C ₆ H ₈ O ₂	sorbic acid (c)	-744.2	-93.4	[152, 333, 462]
C ₆ H 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	brassicidic 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].
brassicic acid (c)—The combustion data of Stohmann and Langbein [474] are the same as Stohmann [461].

6.13. Aliphatic Dicarboxylic Acids

Formula	Compound (State)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₂ H ₂ O ₄	oxalic acid (c, α)	-58.7	-197.7	[19, 208, 348, 377, 457, 470, 481, 550, 564]
C ₂ H ₂ O ₄	oxalic acid (c, β)	-59.0	-197.4	[527]
C ₂ H ₆ O ₆	oxalic acid dihydrate (c)	-52.0	-341.0	[19, 214, 215]
C ₃ H ₄ O ₄	malonic acid (c)	-205.82	-212.96	[269, 271, 377, 457, 470, 550, 564]
C ₄ H ₆ O 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 ₅ H ₈ O ₄	glutaric acid (c)	-514.08	-229.44	[467, 470, 550, 564]
C ₆ H 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₄ H ₆ O ₅	L-malic acid (c)	-317.37	-263.78	[564]
C ₄ H ₆ O ₅	DL-malic acid (c)	-316.88	-264.27	[564]
C ₄ H ₆ O ₆	L-tartaric acid (c)	-274.7	-306.5	[78, 116, 142, 377, 457, 481]
C ₄ H ₆ O ₆	DL-tartaric acid (c)	-272.6	-308.5	[78, 116, 142, 335, 337, 338]
C ₄ H ₆ O ₆	meso-tartaric acid (c)	-275.3	-305.9	[78, 116, 142]
C ₄ H ₈ O ₇	DL-tartaric acid monohydrate (c)	-278	-371	[335, 337, 338]
C ₅ H ₆ O ₅	α -ketoglutaric acid (c)	-429.85	-245.35	[563]
C ₅ H ₈ O ₇	DL-trihydroxyglutaric acid (c)	-388	-356	[156]
C ₆ H ₈ O ₇	citric acid (anhydrous) (c)	-468.6	-369.0	[271, 377, 457, 470, 470, 481, 564]
C ₆ H ₁₀ O ₈	citric acid monohydrate (c)	-466.48	-439.40	[93, 271]
C ₆ H ₁₀ O ₈	allomucic acid (c)	-494	-412	[156]
C ₆ H 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₄ H ₄ O ₄	maleic acid (c)	-323.89	-188.94	[199, 257, 268, 271, 339, 422, 470, 564]
C ₄ H ₄ O ₄	fumaric acid (c)	-318.99	-193.84	[199, 257, 268, 271, 339, 422, 459, 476, 564]
C ₅ H ₆ O ₄	citraconic acid (c)	-478.16	-197.04	[268, 271, 461, 462, 563]
C ₅ H ₆ O ₄	itaconic acid (c)	-474.14	-201.06	[268, 271, 462, 563]
C ₅ H ₆ O ₄	mesaconic acid (c)	-478	-197	[268, 271]
C ₆ H ₆ O ₆	cis-aconitic acid (c)	-476.6	-292.7	[271, 462, 563]
C ₆ H ₆ O ₆	trans-aconitic acid (c)	-474.6	-294.7	[271, 462, 563]
C ₆ H ₈ O ₄	hexa-2-ene-1,6-dioic acid (c)	-629	-209	[462]
C ₆ H ₈ O ₄	hexa-3-ene-1,6-dioic acid (c)	-629	-209	[462]
C ₇ H 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₇ H ₆ O 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 ₇ H ₆ O 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 ₈ H ₆ O ₃	phenylglyoxylic acid (c)	-842.1	-115.3	[325]
C ₈ H ₆ O ₄	<i>o</i> -phthalic acid (c)	-770.44	-186.91	[271, 377, 384, 423, 457, 462, 469, 548]
C ₈ H ₆ O ₄	<i>m</i> -phthalic acid (c)	-765.44	-191.91	[423, 469, 548]

6.16. Aromatic Acids and Phenylated Aliphatic Acids—Continued

Formula	Compound (State)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₈ H ₆ O ₄	<i>p</i> -phthalic acid (c)	-762.30	-195.05	[423, 469]
C ₈ H ₈ O ₂	phenylacetic acid (c)	-930.4	-95.3	[13, 152, 377, 460, 469, 492, 571]
C ₈ H ₈ O ₃	L-mandelic acid (c)	-886.9	-138.8	[460, 480, 574]
C ₈ H ₈ O ₃	DL-mandelic acid (c)	-887.2	-138.5	[460, 480, 574]
C ₈ H ₈ O ₃	phenoxyacetic acid (c)	-902.9	-122.8	[460, 480]
C ₉ H ₁₀ O ₄	DL-phenylglyceric acid (c)	-1009.5	-178.5	[27]

benzoic acid (c)—The selected value was obtained by using $\Delta U_B = -26434\text{ J g}^{-1}$ 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₄ H ₂ O ₃	maleic anhydride (c)	-332.10	-112.42	[271, 336, 337, 338, 344, 564]
C ₄ H ₄ O ₃	succinic anhydride (c)	-369.0	-143.8	[271, 460, 549]
C ₄ H ₆ O 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₂ H ₄ O ₂	methyl formate (g)	-241.0	-83.7	[66, 531]
C ₂ H ₄ O ₂	methyl formate (liq)	-234.1	-90.6	[49, 50, 150, 398]
C ₃ H ₆ O ₂	methyl acetate (liq)	-380.7	-106.4	[407]
C ₆ H ₁₂ O ₂	methyl valerate (liq)	-851.31	-122.89	[3, 176]
C ₇ H ₁₄ O ₂	methyl caproate (liq)	-1007.46	-129.10	[3]
C ₈ H ₁₆ O ₂	methyl enanthate (liq)	-1163.40	-135.53	[3]
C ₉ H 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₈ H ₈ O ₂	methyl benzoate (liq)	-945.9	-79.8	[487]
C ₉ H ₈ O 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₄ H ₆ O ₄	dimethyl oxalate (liq)	-400.2	-181.0	[471, 547]
C ₅ H ₈ O ₄	dimethyl malonate (liq)	-553.3	-190.2	[170, 547]
C ₆ H ₈ O ₄	dimethyl maleate (liq)	-669.4	-168.2	[336, 337, 338]
C ₆ H ₈ O ₄	dimethyl fumarate (liq)	-663.3	-174.3	[336, 337, 338, 471]
C ₆ H ₁₀ O ₄	dimethyl succinate (liq)	-706.3	-199.6	[471, 547]
C ₇ H ₁₂ O ₄	dimethyl glutarate (liq)	-862.3	-205.9	[547]
C ₈ H 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₁₀ H ₁₀ O ₄	dimethyl <i>o</i> -phthalate (liq)	-1120	-162	[471]
C ₁₀ H ₁₀ O ₄	dimethyl <i>m</i> -phthalate (c)	-1111	-171	[471]
C ₁₀ H ₁₀ O ₄	dimethyl <i>p</i> -phthalate (c)	-1112	-170	[471, 460]

6.22. Glyceryl Esters

Formula	Compound (State)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₅ H ₁₀ O ₄	glyceryl-1-acetate (liq)	-594.3	-217.5	[525]
C ₇ H ₁₂ O ₅	glyceryl-1,3-diacetate (liq)	-800.0	-268.2	[525]
C ₉ H 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ 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	tricyclobutylin (liq)	-1847	-247	[516]
C ₁₅ H ₂₀ O ₆	glyceryl tributyrat (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 ₉₈ O ₅	glyceryl dierucate (c)	-6979	-447	[474]
C ₄₇ H ₉₈ 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₁₉ H ₃₂	5 α -androstane (c)	-2805	-75	[340]
C ₁₉ H ₂₆ O ₂	Δ_4 -androstene-3,17-dione (c)	-2572	-103	[340]
C ₁₉ H ₂₈ O ₂	5 α -androstane-3,17-dione (c)	-2613	-130	[340]
C ₁₉ H ₂₈ O ₂	Δ_4 -androstene-3-one-17 β -ol (c) (testosterone)	-2649	-94	[340]
C ₁₉ H ₂₈ O ₂	Δ_5 -androstene-3 β -ol-17-one (c) (<i>trans</i> -dehydroandrosterone)	-2636	-107	[340]
C ₁₉ H ₃₀ O ₂	5 α -androstane-3 α -ol-17-one (c) (androsterone)	-2650	-162	[340]
C ₁₉ H ₃₀ O ₂	5 α -androstane-3 β -ol-17-one (c) (epiandrosterone)	-2660	-152	[340]
C ₁₉ H ₃₀ O ₂	5 α -androstane-3-one-17 β -ol (c)	-2692	-120	[340]
C ₂₁ H ₂₈ O ₅	Δ_4 -pregnene-3,11,20-trione- 17 α ,21-diol (c) (cortisone)	-2676	-255	[340]

6.23. Steroids—Continued

Formula	Compound (State)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ 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-11 β , 17 α ,21-triol (c) (cortisol)	-2744	-256	[340]
C ₂₄ H ₄₂ O ₆	5 β -cholan-24-oic acid-3 α ,7 α , 12 α -triol monohydrate (c)	-3404	-288	[35, 37]
C ₂₇ H ₄₆ O	Δ_5 -cholestene-3 β -ol (c) (cholesterol)	-3978	-133	[45, 46, 340, 583]
C ₂₈ H ₄₈ O	Δ_5 -cholestene-3 β -yl methyl ether (c)	-4117.1	-155.9	[207]
C ₂₈ H ₄₈ O	3:5-cyclocholestan-6 β -yl methyl ether (c)	-4122.8	-150.3	[207]

5 α -androstane-3-one-17 β -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-3 β -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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₃ H ₄ O ₂	β -propiolactone (g)	-351.17	-67.61	[80]
C ₃ H ₄ O ₂	β -propiolactone (liq)	-339.93	-78.85	[80]
C ₄ H ₄ O ₂	β -methylene- β -propiolactone (liq) (diketene)	-457.11	-55.72	[281]
C ₅ H ₆ O ₂	levulinic lactone (liq)	-599.0	-76.2	[44]
C ₅ H ₈ O ₅	D-arabonic acid- γ -lactone (c)	-505.3	-238.2	[497]
C ₆ H ₆ O ₆	D-mannonic-1,4-3,6-dilactone (c)	-514.7	-254.6	[497]
C ₆ H ₈ O ₄	lactide (c)	-653.4	-184.2	[47, 48]
C ₆ H ₈ O ₆	L-ascorbic acid (c)	-559.23	-278.34	[136]
C ₆ H ₈ O ₇	D-glucaric acid-1,4-lactone (c)	-494.4	-343.2	[497]
C ₆ H ₈ O ₇	D-glucaric acid-3,6-lactone (c)	-494.0	-343.6	[497]
C ₆ H ₁₀ O ₅	saccharinic acid lactone (c)	-656.3	-249.6	[463]
C ₆ H ₁₀ O ₆	D-mannonic acid- γ -lactone (c)	-609.7	-296.2	[156, 497]
C ₆ H ₁₀ O ₆	D-galactonic acid- γ -lactone (c)	-607.6	-298.3	[497]
C ₆ H ₁₀ O ₆	L-gulonic acid- γ -lactone (c)	-614.4	-291.5	[156]
C ₆ H ₁₀ O ₆	D-gluconic acid- δ -lactone (c)	-605.6	-300.3	[497]
C ₇ H ₁₀ O ₄	terebic acid (c)	-778	-222	[333, 334, 337, 338]
C ₇ H ₁₂ O ₇	D-gluco-D-gulo-heptonic acid- γ -lactone (c)	-712.7	-355.6	[156, 497]
C ₈ H 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₅ H ₁₀ O ₅	α-D-xylose (c)	-559.0	-252.8	[58, 220, 442]
C ₅ H ₁₀ O ₅	β-D- and β-L-arabinose (c)	-558.99	-252.84	[58, 136, 220, 457, 476, 481]
C ₅ H ₁₀ O ₅	β-D-ribose (c)	-560.67	-251.16	[136, 496]
C ₆ H ₁₀ O ₅	levoglucosan (c)	-676.6	-229.3	[220, 418, 442]
C ₆ H ₁₂ O ₅	D-fucose (c)	-711.5	-262.7	[476]
C ₆ H ₁₂ O ₅	β-L-rhamnose (c)	-717.7	-256.5	[220, 476]
C ₆ H ₁₂ O ₆	α-D-glucose (c)	-669.94	-304.26	[70, 144, 162, 199, 366, 369, 377, 442, 457, 460, 470, 481]
C ₆ H ₁₂ O ₆	β-D-glucose (c)	-671.44	-302.76	[180, 181, 199, 498, 529]
C ₆ H ₁₂ O ₆	α-D-galactose (c)	-670.1	-304.1	[96, 220, 377, 457, 476, 481, 496]
C ₆ H ₁₂ O ₆	L-sorbose (c)	-670.6	-303.6	[96, 476]
C ₆ H ₁₂ O ₆	β-D-fructose (c)	-672.0	-302.2	[96, 144, 476]
C ₆ H ₁₂ O ₆	D-mannose (c)	-672.3	-301.9	[496]
C ₆ H ₁₄ O ₆	α-L-rhamnose monohydrate (c)	-711.2	-331.3	[476]
C ₆ H ₁₄ O ₇	α-D-glucose hydrate (c)	-667.54	-374.97	[180, 181, 199, 529]
C ₇ H ₁₄ O ₆	α-methyl-D-glucopyranoside (c)	-841.8	-294.8	[308, 442, 571]
C ₇ H ₁₄ O ₆	β-methyl-D-glucopyranoside (c)	-840.8	-295.8	[442]
C ₇ H ₁₄ O ₆	β-methyl-D-glucofuranoside (liq)	-849.1	-287.5	[442]
C ₇ H 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, Strepikeev, and Kozina [442] were chosen in preference to the earlier work.

β-D- and β-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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ 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 KClO₃ combustion data of Stohmann [457].

melezitose (c)—Stohmann and Langbein [476] gave the formula, C₁₈H₃₄O₁₇, 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, C₁₈H₃₂O₁₆.

6.28. Heterocyclic Oxygen Compounds

Formula	Compound (State)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₃ H ₄ O ₃	ethylene carbonate (c)	-279.9	-138.9	[433]
C ₃ H ₆ O	oxacyclobutane (g) (trimethylene oxide).	-467.85	-19.25	[349]
C ₄ H ₄ O	furan (g)	-504.60	-8.23	[174, 358]
C ₄ H ₄ O	furan (liq)	-497.99	-14.84	[174, 246]
C ₄ H ₈ O	tetrahydrofuran (g)	-605.44	-44.03	[349]
C ₄ H ₈ O	tetrahydrofuran (liq)	-598.4	-51.1	[88, 442]
C ₄ H ₈ O ₂	glycol acetal (liq)	-558.4	-91.1	[132]
C ₄ H ₈ O ₂	1,3-dioxane (liq)	-559.48	-89.99	[155, 357, 445]
C ₄ H ₈ O ₂	1,4-dioxane (liq)	-564.99	-84.47	[183, 405, 445]
C ₅ H ₄ O ₂	furfural (liq)	-559.1	-47.8	[71, 94, 246, 312]
C ₅ H ₄ O ₃	2-furoic acid (c) (pyromucic acid)	-487.8	-119.1	[71, 246, 318, 344, 460]
C ₅ H ₆ O ₂	furfuryl alcohol (liq)	-609.2	-66.0	[246, 318, 344]
C ₅ H ₈ O	dihydropyran, 4H (liq)	-706.0	-37.5	[88]
C ₅ H ₁₀ O	tetrahydropyran (g)	-758.44	-53.39	[349]
C ₅ H ₁₀ O	tetrahydropyran (liq)	-750.7	-61.1	[88, 440, 442, 445]
C ₅ H ₁₀ O ₂	tetrahydrofurfuryl alcohol (liq)	-707.7	-104.1	[246]
C ₆ H ₁₀ O ₄	erythritol diformal (c)	-744.1	-161.8	[132]
C ₈ H ₁₄ O ₄	erythritol diacetal (c)	-1049	-182	[132]
C ₉ H 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, $\Delta H_c^\circ = -504.45 \pm 0.15$, and -8.39 ± 0.16 kcal mol⁻¹, are in excellent agreement with the value obtained by combining ΔH_c° (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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
CH ₅ N	methylamine (liq)	−253.5	−11.3	[206, 252, 520]
CH ₆ N ₂ O ₃	methylamine nitrate (c)	−214.3	−84.7	[117, 304]
C ₂ H ₇ N	ethylamine (liq)	−409.5	−17.7	[206, 252, 520]
C ₂ H ₇ N	dimethylamine (liq)	−416.7	−10.5	[206, 252, 520]
C ₂ H ₈ N ₂	ethylenediamine (liq)	−446.30	−15.06	[38, 166]
C ₂ H ₈ N ₂ O ₃	ethylamine nitrate (c)	−373.7	−87.7	[117]
C ₂ H ₈ N ₂ O ₃	dimethylamine nitrate (c)	−381.8	−79.6	[117]
C ₂ H ₁₀ N ₄ O ₆	ethylenediamine dinitrate (c)	−373.5	−156.2	[302, 421]
C ₃ H ₉ N	<i>n</i> -propylamine (liq)	−565.31	−24.26	[252, 444, 520]
C ₃ H ₉ N	isopropylamine (liq)	−562.74	−26.83	[444]
C ₃ H ₉ N	trimethylamine (liq)	−578.6	−11.0	[206, 252, 520]
C ₃ H ₁₀ N ₂	1,2-propanediamine (liq)	−600.35	−23.38	[166]
C ₃ H ₁₀ N ₂ O ₃	trimethylamine nitrate (c)	−549.6	−74.1	[117]
C ₄ H ₁₁ N	<i>n</i> -butylamine (liq)	−721.42	−30.52	[145, 252, 520]
C ₄ H ₁₁ N	isobutylamine (liq)	−720.25	−31.68	[166, 252]
C ₄ H ₁₁ N	sec.-butylamine (liq)	−719.07	−32.87	[145, 252]
C ₄ H ₁₁ N	tert.-butylamine (liq)	−715.97	−35.97	[145, 252, 444, 520]
C ₄ H ₁₁ N	diethylamine (liq)	−727.2	−24.7	[206, 252, 323, 520]
C ₄ H ₁₂ N ₂	1,2-butanediamine (liq)	−757.35	−28.74	[166]
C ₄ H ₁₂ N ₂	2-methyl-1,2-propanediamine (liq)	−754.09	−32.00	[166]
C ₄ H ₁₂ N ₂ O ₃	diethylamine nitrate (c)	−686.0	−100.1	[117]
C ₆ H ₁₅ N	triethylamine (liq)	−1044.6	−32.1	[206, 249, 252, 323, 520]
C ₆ H ₁₆ N ₂ O ₃	triethylamine nitrate (c)	−1011.9	−98.9	[117]
C ₉ H ₂₁ N	tri- <i>n</i> -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] ($\Delta H_c^\circ = -1046.15 \text{ kcal mol}^{-1}$, $\Delta H_f^\circ = -30.54 \text{ kcal mol}^{-1}$) are in reasonable agreement with the selection.

6.30. Aromatic Amines

Formula	Compound (State)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₆ H ₇ N	aniline (liq)	-810.96	+7.55	[8, 104, 179, 195, 252, 353, 355, 460, 464, 465, 508, 509, 520, 551]
C ₆ H ₈ N ₂ O ₃	aniline nitrate (c)	-793.9	-43.7	[117, 568]
C ₇ H ₉ N	<i>N</i> -methylaniline (liq)	-973.5	+7.7	[160, 354, 355, 551]
C ₈ H ₁₁ N	<i>N,N</i> -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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
CH ₃ NO	formamide (liq)	-135.8	-60.7	[400, 489, 491]
C ₂ H ₃ NO ₃	oxamic acid (c)	-130.2	-160.4	[293, 464, 465]
C ₂ H ₄ N ₂ O ₂	oxamide (c)	-201.7	-123.0	[464, 465, 526]
C ₂ H ₅ NO	acetamide (c)	-282.9	-76.0	[51, 87, 489, 491]
C ₃ H ₆ N ₂ O ₂	malonamide (c)	-356.6	-130.5	[464, 465, 524]
C ₃ H ₇ NO	propionamide (c)	-439.6	-81.7	[51, 489, 491]
C ₃ H ₇ NO	<i>N,N</i> -dimethylformamide (liq)	-464.1	-57.2	[308]
C ₃ H ₇ NO ₂	ethylcarbamate (c) (urethane)	-396.9	-124.4	[464, 465]
C ₄ H ₇ NO ₂	diacetamide (c)	-498	-117	[347]
C ₄ H ₈ N ₂ O ₂	succinamide (c)	-510.6	-138.9	[464, 465, 526]
C ₄ H ₈ N ₂ O ₄	<i>L</i> -tartramide (c)	-426.6	-222.9	[116, 526]
C ₄ H ₈ N ₂ O ₄	meso-tartramide (c)	-426.0	-223.5	[116]
C ₄ H ₉ NO	<i>n</i> -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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₇ H ₇ NO	benzamide (c)	-849.04	-48.42	[8, 51, 104, 489, 491]
C ₇ H ₇ NO	formanilide (c)	-861.2	-36.2	[489, 491]
C ₈ H ₈ N ₂ O ₂	phthalamide (c)	-921.3	-104.4	[464, 465]
C ₈ H ₉ NO	acetanilide (c)	-1009.5	-50.3	[51, 489, 491, 554]

6.32. Aromatic Amides—Continued

Formula	Compound (State)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
CH ₄ N ₂ O	urea (c)	-150.97	-79.71	[67, 68, 144, 194, 242, 283, 410, 411, 457, 460, 475, 481]
CH ₅ N ₃	guanidine (c)	-251.45	-13.39	[234]
CH ₅ N ₃ O ₄	urea nitrate (c)	-130.0	-134.8	[302, 421]
CH ₅ N ₅ O ₂	nitroaminoguanidine (c)	-270.13	+5.29	[301]
CH ₆ N ₄ O ₃	guanidine nitrate (c)	-206.5	-92.5	[241, 292, 293]
CH ₈ N ₆ O ₃	<i>sym</i> -diaminoguanidine nitrate (c)	-329.74	-37.57	[301]
C ₂ H ₄ N ₂ O ₂	formylurea (c)	-207	-118	[289, 293]
C ₂ H ₄ N ₄ O ₂	azodicarbamide (c)	-254.83	-69.90	[566]
C ₂ H ₅ N ₅ O ₃	1-formamido-2-nitro-guanidine (c)	-323.8	-35.1	[566]
C ₂ H ₆ N ₄ O ₂	hydrazodicarbamide (c)	-273.86	-119.19	[566]
C ₂ H ₇ N ₅ O ₄	guanylurea nitrate (c)	-325.1	-102.1	[446]
C ₃ H ₆ N ₂ O ₃	hydantoic acid (c) (ureido-acetic acid)	-308	-179	[307]
C ₃ H ₇ N ₅ O ₃	1-acetamido-2-nitro-guanidine (c)	-475.0	-46.3	[566]
C ₃ H ₉ N ₅ O ₄	acetamidoguanidine nitrate (c)	-471.5	-118.1	[566]
C ₃ H ₁₂ N ₆ O ₃	guanidine carbonate (c)	-459.95	-232.10	[194, 306]
C ₄ H ₉ N ₃ O ₂	creatinine (c)	-555.46	-128.16	[144, 198, 475]
C ₄ H ₁₁ N ₃ O ₃	creatinine 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].

creatinine (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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₂ H ₅ NO ₂	glycine (c)	-232.67	-126.22	[43, 144, 152, 200, 457, 475, 481, 535, 571]
C ₂ H ₆ N ₂ O ₅	glycine nitrate (c)	-218.9	-174.1	[117]
C ₃ H ₇ NO ₂	L-alanine (c)	-387.30	-133.96	[43, 144, 198, 535, 571]
C ₃ H ₇ NO ₂	DL-alanine (c)	-386.71	-134.55	[148, 200, 460, 475, 571]
C ₃ H ₇ NO ₂	sarcosine (c)	-400.1	-121.2	[85, 475]
C ₃ H ₇ NO ₂ S	L-cysteine (c)	-540.5	-124.6	[20, 81, 197, 501]

6.34. Aliphatic Amino Acids—Continued

Formula	Compound (State)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₃ H ₇ NO ₃	L-isoserine (c)	-343.5	-177.8	[152, 571]
C ₃ H ₇ NO ₃	L-serine (c)	-347.7	-173.6	[201]
C ₄ H ₇ NO ₄	L-aspartic acid (c)	-382.84	-232.47	[43, 144, 152, 198, 331, 460, 475]
C ₄ H ₇ NO ₄	diglycolamidic acid (c)	-395.8	-219.5	[462, 479]
C ₄ H ₈ N ₂ O ₃	L-asparagine (c)	-460.97	-188.50	[43, 198, 457, 460, 475, 481]
C ₄ H ₉ NO ₂	γ -aminobutyric acid (c)	-545.5	-138.1	[495]
C ₄ H ₉ NO ₃	DL- and L-threonine (c)	-502.2	-181.4	[369, 535]
C ₄ H ₁₀ N ₂ O ₄	L-asparagine monohydrate (c)	-458.26	-259.52	[144, 198]
C ₅ H ₉ NO ₂	DL-proline (c)	-652.0	-125.7	[369]
C ₅ H ₉ NO ₃	L-hydroxyproline (c)	-619.6	-158.1	[369]
C ₅ H ₉ NO ₄	L-glutamic acid (c)	-536.2	-241.5	[144, 152, 198, 331, 536]
C ₅ H ₁₀ N ₂ O ₃	L-glutamine (c)	-614.5	-197.3	[536]
C ₅ H ₁₁ NO ₂	δ -aminovaleric acid (c)	-701.5	-144.5	[495]
C ₅ H ₁₁ NO ₂	DL- and L-valine (c)	-697.8	-148.2	[439, 536, 571]
C ₅ H ₁₁ NO ₂ S	L-methionine (c)	-809.5	-180.4	[535]
C ₅ H ₁₂ N ₂ O ₂	DL-ornithine (c)	-724.1	-156.0	[369]
C ₆ H ₉ NO ₆	nitrilotriacetic acid (c)	-559.2	-312.5	[462, 479]
C ₆ H ₁₃ N ₂ O ₄ S ₂	L-cystine (c)	-1016.3	-245.7	[20, 81, 144, 197, 501]
C ₆ H ₁₃ NO ₂	α -aminocaproic acid (c) (norleucine)	-855.6	-152.7	[439, 495]
C ₆ H ₁₃ NO ₂	γ -aminocaproic acid (c)	-853.9	-154.5	[495]
C ₆ H ₁₃ NO ₂	δ -aminocaproic acid (c)	-854.6	-153.7	[495]
C ₆ H ₁₃ NO ₂	ϵ -aminocaproic acid (c)	-855.6	-152.7	[495]
C ₆ H ₁₃ NO ₂	D-leucine (c)	-856.39	-151.97	[200]
C ₆ H ₁₃ NO ₂	L-leucine (c)	-856.39	-151.97	[43, 152, 200, 460, 475, 536]
C ₆ H ₁₃ NO ₂	DL-leucine (c)	-855.62	-152.74	[200]
C ₆ H ₁₃ NO ₂	DL- and L-isoleucine (c)	-856.5	-151.8	[369, 535]
C ₆ H ₁₄ N ₂ O ₂	DL-lysine (c)	-880.3	-162.2	[369]
C ₆ H ₁₄ N ₄ O ₂	L-arginine (c)	-893.85	-148.66	[200]
C ₇ H ₁₃ NO ₃	N-formyl-DL-leucine (c)	-880.3	-222.1	[571]
C ₇ H ₁₅ NO ₂	ζ -aminoanthranic acid (c)	-1011.1	-159.6	[495]
C ₉ H ₁₉ NO ₂	ω -aminopelargonic acid (c)	-1321.4	-174.1	[495]
C ₁₀ H ₁₆ N ₂ O ₈	ethylenediaminetetraacetic acid (c)	-1066.5	-420.5	[1]
C ₁₂ H ₂₆ N ₂ O ₄	hexamethylene-1,6-diamine- adipic acid adduct (c)	-1711.2	-305.5	[495]
C ₁₄ H ₂₃ N ₃ O ₁₀	diethylenetriamine- pentaacetic acid (c)	-1570.5	-531.8	[1]
C ₁₄ H ₃₀ N ₂ O 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 H₂SO₄ · 115H₂O(lig), and $\Delta H_f^\circ[\text{H}_2\text{SO}_4 \cdot 115\text{H}_2\text{O}(\text{lig})] = -212.192\text{ kcal mol}^{-1}$.

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 ΔH_f° 298 [L-threonine (c)] of $-193.11 \text{ kcal mol}^{-1}$ 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 $\text{H}_2\text{SO}_4 \cdot 115\text{H}_2\text{O}(\text{liq})$, and $\Delta H_f^\circ[\text{H}_2\text{SO}_4 \cdot 115\text{H}_2\text{O}(\text{liq})] = -212.192 \text{ kcal mol}^{-1}$.

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 $\text{H}_2\text{SO}_4 \cdot 115\text{H}_2\text{O}(\text{liq})$, and $\Delta H_f^\circ[\text{H}_2\text{SO}_4 \cdot 115\text{H}_2\text{O}(\text{liq})] = -212.192 \text{ kcal mol}^{-1}$.

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 ΔH_f° 298 [L-isoleucine (c)] of $-152.9 \text{ kcal mol}^{-1}$ 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)	ΔH_c° 298 K kcal mol ⁻¹	ΔH_f° 298 K kcal mol ⁻¹	Reference
$\text{C}_7\text{H}_7\text{NO}_2$	<i>o</i> -aminobenzoic acid (c)	-801.7	-95.8	[250]
$\text{C}_7\text{H}_7\text{NO}_2$	<i>m</i> -aminobenzoic acid (c)	-799.3	-98.2	[250]
$\text{C}_7\text{H}_7\text{NO}_2$	<i>p</i> -aminobenzoic acid (c)	-798.7	-98.8	[250]
$\text{C}_8\text{H}_9\text{NO}_2$	<i>N</i> -phenyl glycine (c)	-963.6	-96.2	[152]
$\text{C}_8\text{H}_9\text{NO}_2$	α -phenyl glycine (c)	-956.6	-103.2	[152, 244]
$\text{C}_9\text{H}_9\text{NO}_3$	hippuric acid (c)	-1008.25	-145.63	[100, 104, 144, 148, 188, 193, 196, 450, 457, 460, 475, 481, 492, 557]
$\text{C}_9\text{H}_{11}\text{NO}_2$	DL- and L-phenylalanine (c)	-1110.3	-111.9	[85, 152, 535]
$\text{C}_9\text{H}_{11}\text{NO}_3$	L-tyrosine (c)	-1058.8	-163.4	[43, 144, 200, 331]
$\text{C}_{10}\text{H}_{11}\text{NO}_3$	phenaceturic acid (c)	-1165.2	-151.0	[490, 492]
$\text{C}_{10}\text{H}_{11}\text{NO}_3$	DL-benzoylalanine (c)	-1168.3	-147.9	[490, 492]
$\text{C}_{10}\text{H}_{11}\text{NO}_3$	benzoyl sarcosine (c)	-1180.5	-135.7	[490, 492]
$\text{C}_{10}\text{H}_{11}\text{NO}_3$	<i>p</i> -toluyl glycine (c)	-1167.7	-148.5	[490, 492]
$\text{C}_{10}\text{H}_{11}\text{NO}_3$	<i>m</i> -toluyl glycine (c)	-1167.4	-148.8	[490, 492]
$\text{C}_{10}\text{H}_{11}\text{NO}_3$	<i>o</i> -toluyl glycine (c)	-1167.9	-148.3	[490, 492]
$\text{C}_{10}\text{H}_{11}\text{NO}_4$	anisoyl glycine (c)	-1135.3	-180.9	[490, 492]
$\text{C}_{11}\text{H}_{12}\text{N}_2\text{O}_2$	L-tryptophane (c)	-1344.6	-99.8	[535]
$\text{C}_{11}\text{H}_{13}\text{NO}_3$	<i>o</i> -toluyl alanine (c)	-1322.1	-156.5	[490, 492]
$\text{C}_{11}\text{H}_{13}\text{NO}_3$	<i>p</i> -toluyl alanine (c)	-1319.6	-159.0	[490, 492]
$\text{C}_{12}\text{H}_{15}\text{NO}_4$	DL-phenylalanine- <i>N</i> -carboxylic acid dimethyl ester (c)	-1456.7	-184.3	[85]
$\text{C}_{16}\text{H}_{11}\text{NO}_2$	benzalhippuric acid azlactone (c)	-1850.0	-30.5	[152]
$\text{C}_{16}\text{H}_{13}\text{NO}_3$	benzalhippuric acid (c)	-1846.3	-102.6	[152]
$\text{C}_{16}\text{H}_{15}\text{NO}_3$	benzoylphenylalanine (c)	-1887.6	-129.6	[152]
$\text{C}_{17}\text{H}_{19}\text{NO}_2$	ethyl β -anilino- β -phenyl propionate (c)	-2165.1	-82.8	[370]
$\text{C}_{36}\text{H}_{44}\text{N}_2\text{O}_{10}$	L(+)-leucine methyl ester salt of (-)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3') (c)	-4358	-531	[243]
$\text{C}_{36}\text{H}_{44}\text{N}_2\text{O}_{10}$	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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₄ H ₅ NO ₃	sarcosine- <i>N</i> -carboxylic acid anhydride (c)	-402.9	-144.1	[85]
C ₄ H ₆ N ₂ O ₂	glycine anhydride (c)	-475.1	-106.0	[152, 244, 571]
C ₆ H ₁₀ N ₂ O ₂	alanine anhydride (c)	-777.9	-128.0	[152, 244, 300, 571]
C ₆ H ₁₀ N ₂ O ₄	serine anhydride (c)	-696.4	-209.5	[368]
C ₇ H ₁₂ N ₂ O ₂	glycylvalyl anhydride (c)	-947.7	-120.5	[585]
C ₈ H ₁₄ N ₂ O ₂	valylalanyl anhydride (c)	-1107.3	-123.3	[368]
C ₁₀ H ₉ NO ₃	phenylalanine- <i>N</i> -carboxylic acid anhydride (c)	-1115.6	-132.3	[85]
C ₁₁ H ₁₂ N ₂ O ₂	glycylphenylalanyl anhydride (c)	-1361.6	-82.9	[368]
C ₁₁ H ₁₂ N ₂ O ₃	glycyltyrosyl anhydride (c)	-1321.7	-122.8	[368]
C ₁₁ H ₂₀ N ₂ O ₂	valylleucyl anhydride (c)	-1567.6	-150.1	[368]
C ₁₂ H ₁₄ N ₂ O ₂	alanylphenylalanyl anhydride (c)	-1517.5	-89.3	[368]
C ₁₂ H ₂₂ N ₂ O ₂	leucine anhydride (c)	-1720.1	-160.0	[152]
C ₁₄ H ₁₈ N ₂ O ₂	valylphenylalanyl anhydride (c)	-1837.2	-94.3	[368]
C ₁₈ H ₁₈ N ₂ O 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 phenylalanine-*N*-carboxylic acid anhydride are not diketopiperazines.

6.37. Peptides

Formula	Compound (State)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₄ H ₈ N ₂ O ₃	glycylglycine (c)	-470.95	-178.51	[152, 196, 244]
C ₅ H ₈ N ₂ O ₅	glycylglycine- <i>N</i> -carboxylic acid (c)	-470.5	-273.0	[152, 571]
C ₅ H ₁₀ N ₂ O ₃	DL-alanylglycine (c)	-626.19	-185.64	[196]
C ₆ H ₁₁ N ₃ O ₄	diglycylglycine (c)	-709.2	-230.8	[571]
C ₆ H ₁₂ N ₂ O ₃	ethyl glycylglycinate (c)	-803.7	-170.5	[152, 244]
C ₆ H ₁₂ N ₂ O ₅	serylserine (c)	-692.4	-281.8	[367]
C ₇ H ₁₄ N ₂ O ₃	glycylvaline (c)	-936.6	-200.0	[367]
C ₈ H ₁₄ N ₄ O ₅	triglycylglycine (c)	-945.9	-284.7	[571]
C ₈ H ₁₆ N ₂ O ₃	DL-leucylglycine (c)	-1093.86	-205.7	[196, 571]
C ₉ H ₁₆ N ₂ O ₅	α -carbethoxyglycyl glycine ethyl ester (c)	-1117.7	-275.3	[152]
C ₉ H ₁₆ N ₂ O ₅	β -carbethoxyglycylglycine ethyl ester (c)	-1089.5	-303.5	[152]
C ₁₀ H ₁₉ N ₃ O ₄	leucylglycylglycine (c)	-1329.9	-259.6	[152]
C ₁₁ H ₁₂ N ₂ O ₄	hippurylglycine (c)	-1245.92	-198.54	[196]
C ₁₁ H ₁₄ N ₂ O ₃	glycylphenylalanine (c)	-1348.8	-163.9	[367]

6.37. Peptides—Continued

Formula	Compound (State)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₁₂ H ₁₆ N ₂ O ₃	alanylphenylalanine (c)	-1505.0	-170.2	[367]
C ₁₄ H ₁₉ N ₃ O ₄	glycylalanylphenylalanine (c)	-1743.7	-222.0	[367]
C ₁₄ H ₂₀ N ₂ O 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₈ H 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 ₂ O	cinchonidine (c)	-2545.5	+7.1	[52, 54]
C ₁₉ H ₂₂ N ₂ O	cinchonine (c)	-2545.8	+7.4	[52, 54]
C ₁₉ H ₂₄ N ₂ O	cinchonamine (c)	-2596.3	-10.4	[52, 54]
C ₁₉ H ₂₅ N ₃ O 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 ₂ O ₂	quinidine (c)	-2662.5	-38.3	[52, 53]
C ₂₀ H ₂₄ N ₂ O ₂	quinine (c)	-2663.7	-37.1	[52, 53]
C ₂₁ H ₂₂ N ₂ O 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 ₂ O 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 stereoisomers, 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)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
CH ₂ N ₄	tetrazole (c)	-219.0	+56.7	[301]
CH ₂ N ₄ O	5-hydroxytetrazole (c)	-163.9	+1.5	[566]
CH ₃ N ₅	5-aminotetrazole (c)	-246.2	+49.7	[301]
CH ₄ N ₆ O ₃	5-aminotetrazole nitrate (c)	-224.1	-6.6	[301]
C ₂ HN ₅	5-cyanotetrazole (c)	-318.3	+96.1	[566]
C ₂ H ₂ N ₆	3-azido-s-triazole (c)	-361.9	+105.5	[135]
C ₂ H ₃ N ₇	4-amino-3-azido-s-triazole (c)	-427.1	+136.5	[135]
C ₂ H ₄ N ₄	3-amino-1,2,4-triazole (c)	-343.1	+18.4	[566]
C ₂ H ₄ N ₄ O	5-methoxytetrazole (c)	-341.3	+16.6	[566]
C ₂ H ₄ N ₁₀	5,5'-hydrazotetrazole (c)	-459.8	+135.1	[301]
C ₂ H ₅ N	ethylenimine (liq)	-380.86	+21.97	[324]
C ₂ H ₅ N ₅	1-methyl-5-aminotetrazole (c)	-405.14	+46.25	[565, 566]
C ₂ H ₅ N ₅	2-methyl-5-aminotetrazole (c)	-409.3	+50.4	[565, 566]
C ₂ H ₅ N ₅	5-methylaminotetrazole (c)	-407.2	+48.4	[566]
C ₂ H ₅ N ₇	5-guanylamintetrazole (c)	-399.4	+40.5	[301]
C ₂ H ₅ N ₅ O ₃	3-amino-1,2,4-triazole nitrate (c)	-318.0	-40.9	[566]

6.39. Heterocyclic Nitrogen Compounds – Continued

Formula	Compound (State)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₂ H ₈ N ₁₀ O	1-(5-tetrazolyl)-4-guanyltetra- zene monohydrate (c)	-506.5	+45.2	[566]
C ₃ H ₂ N ₂ O ₃	parabanic acid (c)	-212.5	-138.0	[290, 293]
C ₃ H ₄ N ₂	imidazole (c)	-433.3	+14.5	[24]
C ₃ H ₄ N ₂	pyrazole (c)	-447.1	+28.3	[24]
C ₃ H ₄ N ₂ O ₂	hydantoin (c)	-311.6	-107.2	[307]
C ₃ H ₄ N ₆	3-azido-5-methyl-s-triazole (c)	-512.6	+93.8	[135]
C ₃ H ₅ N ₅ O	5-acetamidotetrazole (c)	-451.7	-1.2	[301]
C ₃ H ₅ N ₇	4-amino-3-azido-5-methyl-s- triazole (c)	-568.6	+115.6	[135]
C ₃ H ₆ N ₄	1,5-dimethyl tetrazole (c)	-532.2	+45.1	[301]
C ₃ H ₆ N ₄ O	1,4-dimethyl-5-tetrazolone (c)	-480.5	-6.6	[566]
C ₃ H ₆ N ₆	melamine (c)	-469.8	-17.3	[113, 414, 525]
C ₃ H ₇ N ₅	5-dimethylaminotetrazole (c)	-564.9	+43.6	[566]
C ₃ H ₇ N ₅ O ₃	3-amino-5-methyl-1,2,4- triazole nitrate (c)	-466.7	-54.6	[566]
C ₃ H ₈ N ₆ O ₃	1,3-dimethyl-5-imino- tetrazole nitrate (c)	-554.1	-1.3	[566]
C ₄ H ₄ N ₂	pyrazine (g)	-559.69	+46.86	[533]
C ₄ H ₄ N ₂	pyrazine (c)	-546.24	+33.41	[533]
C ₄ H ₄ N ₂	pyridazine (g)	-579.35	+66.52	[533]
C ₄ H ₄ N ₂	pyridazine (liq)	-566.57	+53.74	[533]
C ₄ H ₄ N ₂	pyrimidine (g)	-559.82	+46.99	[533]
C ₄ H ₄ N ₂	pyrimidine (liq)	-547.87	+35.04	[533]
C ₄ H ₄ N ₂ O ₃	barbituric acid (c)	-360.6	-152.2	[152, 294]
C ₄ H ₄ N ₂ O ₄	dialuric acid (c)	-198.4	-314.4	[294]
C ₄ H ₄ N ₂ O ₅	alloxan monohydrate (c)	-273.76	-239.08	[288, 294, 456]
C ₄ H ₅ N	pyrrole (g)	-572.87	+25.88	[424]
C ₄ H ₅ N	pyrrole (liq)	-562.07	+15.08	[45, 424]
C ₄ H ₅ N ₃ O ₃	uramil (c)	-378.8	-168.2	[294]
	(5-aminobarbituric acid)			
C ₄ H ₆ N ₂ O ₂	5-methyl hydantoin (c)	-464.8	-116.3	[524]
C ₄ H ₆ N ₂ O ₃	allantoin (c)	-409.64	-171.51	[144, 288, 293, 456]
C ₄ H ₆ N ₆	3-azido-5-ethyl-s-triazole (c)	-668.5	+87.4	[135]
C ₄ H ₆ N ₈	1,2-di-(5-tetrazolyl)ethane (c)	-687.3	+106.2	[566]
C ₄ H ₆ N ₁₀	<i>cis</i> -1,1'-dimethyl-5,5'-azotet- razole (c)	-769.7	+188.6	[566]
C ₄ H ₆ N ₁₀	<i>trans</i> -1,1'-dimethyl-5,5'-azotet- razole (c)	-770.5	+189.3	[566]
C ₄ H ₆ N ₁₀	2,2'-dimethyl-5,5'-azotetra- zole (c)	-761.5	+180.3	[566]
C ₄ H ₇ NO	α -pyrrolidone (c)	-547.0	-68.3	[494]
C ₄ H ₇ N ₃ O	creatinine (c)	-558.54	-56.77	[144, 198]
C ₄ H ₇ N ₅	1-allyl-5-aminotetrazole (c)	-678.7	+63.4	[566]
C ₄ H ₇ N ₅	2-allyl-5-aminotetrazole (c)	-682.9	+67.6	[566]
C ₄ H ₇ N ₇	4-amino-3-azido-5-ethyl-s- triazole (c)	-733.8	+118.5	[135]
C ₄ H ₇ N ₅ O ₂	5-tetrazolylurethan (c)	-562.7	-52.6	[301]
C ₄ H ₉ N	pyrrolidine (g)	-682.73	-0.89	[296]
C ₄ H ₉ N	pyrrolidine (liq)	-673.75	-9.87	[185, 296]
C ₄ H ₁₀ N ₂	piperazine (c)	-706.88	-10.90	[23]
C ₄ H ₂₂ N ₂ O ₆	piperazine hexahydrate (c)	-690.9	-436.8	[36, 38]
C ₅ H ₄ N ₄ O	hypoxanthine (c) (6-oxypurine)	-580.65	-26.24	[39, 40, 456]
C ₅ H ₄ N ₄ O	8-oxypurine (c)	-591.4	-15.4	[39, 40]
C ₅ H ₄ N ₄ O ₂	xanthine (c)	-516.39	-90.49	[45, 46, 456]
C ₅ H ₄ N ₄ O ₃	isouric acid (c)	-459.0	-147.9	[294]
C ₅ H ₄ N ₄ O ₃	uric acid (c)	-459.16	-147.73	[144, 287, 294, 456, 457, 460, 475, 481]
C ₅ H ₅ N	pyridine (g)	-674.65	+33.61	[121, 188]

6.39. Heterocyclic Nitrogen Compounds—Continued

Formula	Compound (State)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₅ H ₅ N	pyridine (liq)	-665.00	+23.96	[111, 121, 130, 131, 188, 493, 512]
C ₅ H ₅ NO	pyrrolaldehyde (c)	-616.3	-24.8	[453]
C ₅ H ₅ N ₅	adenine (c)	-664.25	+23.21	[456]
C ₅ H ₅ N ₅ O	guanine (c)	-597.33	-43.72	[456, 475]
C ₅ H ₆ N ₂ O	pyrrolaldoxime (c)	-678.9	+3.7	[453]
C ₅ H ₆ N ₂ O ₂	4-methyluracil (c)	-566.0	-109.2	[152]
C ₅ H ₆ N ₂ O ₂	thymine (c) (5-methyl uracil)	-563.3	-111.9	[152]
C ₅ H ₆ N ₂ O ₃	dimethyl parabanic acid (c)	-538.2	-137.0	[291, 293]
C ₅ H ₆ N ₄ O ₄	pseudouric acid (c)	-453.5	-221.7	[294]
C ₅ H ₇ N ₃	2,6-diaminopyridine (c)	707.9	1.5	[143, 572]
C ₅ H ₈ N ₂ O ₂	5,5-dimethyl hydantoin (c)	-617.1	-126.4	[300, 524]
C ₅ H ₈ N ₂ O ₂	4-methylhydrouracil (c)	-618.0	-125.5	[152]
C ₅ H ₈ N ₄ O ₃	methyl allantoin (c) (pyvurile)	-566.6	-177.0	[293]
C ₅ H ₉ N	1,2,5,6-tetrahydropyridine (liq)	-785.7	+8.0	[23]
C ₅ H ₉ NO	α -piperidone (c)	-704.4	-73.3	[494]
C ₅ H ₉ NO	N-methylpyrrolidone (liq)	-715.03	-62.64	[240]
C ₅ H ₁₁ N	piperidine (liq)	-824.94	-21.05	[23, 130, 131]
C ₆ H ₄ N ₂	3-cyanopyridine (c)	-747.17	+46.23	[413, 414]
C ₆ H ₅ NO ₂	picolinic acid (c)	-651.4	-83.7	[579]
C ₆ H ₅ N ₃	benzotriazole (c)	-794.84	+59.74	[147]
C ₆ H ₆ N ₄	7-methylpurine (c)	-820.6	+51.3	[39, 40]
C ₆ H ₆ N ₄ O	7-methylhypoxanthine (c)	-759.4	-9.9	[39, 40]
C ₆ H ₇ N	2-methylpyridine (g)	-827.46	+24.05	[121, 426]
C ₆ H ₇ N	2-methylpyridine (liq)	-817.24	+13.83	[111, 121, 408, 426]
C ₆ H ₇ N	3-methylpyridine (g)	-829.71	+26.30	[121, 425]
C ₆ H ₇ N	3-methylpyridine (liq)	-818.98	+15.57	[111, 121, 408, 425]
C ₆ H ₇ N	4-methylpyridine (g)	-827.85	+24.44	[121]
C ₆ H ₇ N	4-methylpyridine (liq)	-816.99	+13.58	[111, 121, 408]
C ₆ H ₁₀ N ₂ O ₂	5-methyl-5-ethyl hydantoin (c)	-770.9	-135.0	[524]
C ₆ H ₁₀ N ₁₀	2,2'-diethyl-5,5'-azotetrazole (c)	-1062.5	+156.6	[566]
C ₆ H ₁₁ NO	ϵ -caprolactam (c)	-861.4	-78.6	[494]
C ₆ H ₁₁ NO	N-methyl piperidone (liq)	-870.04	-70.00	[240]
C ₆ H ₁₂ N ₂	triethylenediamine (c)	-970.8	-3.4	[346]
C ₆ H ₁₂ N ₄	hexamethylenetetramine (c)	-1002.9	+28.7	[14, 15, 125, 127, 133]
C ₆ H ₁₄ N ₆ O ₆	hexamethylenetetramine dinitrate (c)	-953.9	-88.6	[125, 127, 133]
C ₇ H ₆ N ₄	1-phenyltetrazole (c)	-949.8	+86.5	[301]
C ₇ H ₆ N ₄	5-phenyltetrazole (c)	-933.3	+70.0	[301]
C ₇ H ₆ N ₄ O	1-phenyl-5-hydroxytetrazole (c)	-890.0	+26.7	[301]
C ₇ H ₇ N	2-vinylpyridine (liq)	-934.7	+37.2	[18]
C ₇ H ₇ N ₅	1-phenyl-5-aminotetrazole (c)	-971.8	+74.3	[566]
C ₇ H ₇ N ₅	5-phenylaminotetrazole (c)	-970.4	+72.9	[566]
C ₇ H ₈ N ₄ O ₂	theobromine (c)	-845.2	-86.4	[291, 294]
C ₇ H ₉ N	2-ethylpyridine (liq)	-964.6	-1.2	[18]
C ₇ H ₉ N	2,3-dimethylpyridine (liq)	-970.40	+4.62	[122]
C ₇ H ₉ N	2,4-dimethylpyridine (liq)	-969.63	+3.85	[122]
C ₇ H ₉ N	2,5-dimethylpyridine (liq)	-970.23	+4.45	[121, 122]
C ₇ H ₉ N	2,6-dimethylpyridine (liq)	-968.80	+3.02	[111, 121, 122]
C ₇ H ₉ N	3,4-dimethylpyridine (liq)	-970.14	+4.36	[122]
C ₇ H ₉ N	3,5-dimethylpyridine (liq)	-971.14	+5.36	[122]

6.39. Heterocyclic Nitrogen Compounds—Continued

Formula	Compound (State)	$\Delta H_c^\circ 298\text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298\text{ K}$ kcal mol ⁻¹	Reference
C ₇ H ₁₁ N ₅	1-allyl-5-allylaminotetrazole (c)	-1117.8	+83.7	[566]
C ₇ H ₁₁ N ₅	5-diallylaminotetrazole (c)	-1118.0	+83.9	[566]
C ₇ H ₁₃ NO	<i>N</i> -methylcaprolactam (liq)	-1029.1	-73.3	[240]
C ₇ H ₁₃ NO	5-methylcaprolactam (c)	-1015.5	-86.9	[494]
C ₇ H ₁₃ NO	7-methylcaprolactam (c)	-1015.9	-86.5	[494]
C ₇ H ₁₃ NO	ζ-enantholactam (c)	-1019.2	-83.2	[494]
C ₈ H ₅ NO ₂	isatin (c)	-860.5	-62.7	[5, 453]
C ₈ H ₆ N ₄ O ₆	hydurilic acid (c)	-658.2	-299.2	[294]
C ₈ H ₆ N ₆	3-azido-5-phenyl-s-triazole (c)	-1084.5	+127.1	[135]
C ₈ H ₇ N	indole (c)	-1021.3	+29.8	[45, 46, 452]
C ₈ H ₇ NO	oxindole (c)	-950.3	-41.2	[45, 46]
C ₈ H ₇ NO ₂	dioxindole (c)	-914.6	-76.9	[5]
C ₈ H ₇ N ₇	4-amino-3-azido-5-phenyl-s-triazole (c)	-1151.0	+159.5	[135]
C ₈ H ₈ N ₄	1-methyl-5-phenyltetrazole (c)	-1095.6	+69.9	[566]
C ₈ H ₈ N ₄	1-phenyl-5-methyltetrazole (c)	-1095.6	+69.9	[301, 566]
C ₈ H ₈ N ₄	2-phenyl-5-methyltetrazole (c)	-1091.3	+65.7	[301]
C ₈ H ₉ N ₆ O ₆	murexide (c)	-736.0	-289.7	[294]
C ₈ H ₁₀ N ₄ O ₂	caffeine (c) (methyl theobromine)	-1017.8	-76.2	[291, 294, 475]
C ₈ H ₁₀ N ₄ O ₁₀	alloxantin dihydrate (c)	-583.7	-510.3	[288, 294]
C ₈ H ₁₂ N ₂ O ₃	diethylbarbituric acid (c) (veronal)	-983.6	-178.7	[152]
C ₉ H ₇ N	quinoline (liq)	-1122.9	+37.3	[128, 131]
C ₉ H ₇ N	isoquinoline (c)	-1123.5	+37.9	[129, 313]
C ₉ H ₇ NO	8-hydroxyquinoline (c)	-1065.7	-19.9	[499, 500, 570]
C ₉ H ₈ N ₂ O	di-α-pyrrolyketone (c)	-1115.0	-4.7	[452]
C ₉ H ₉ N	α-methylindole (c)	-1168.4	+14.5	[45, 46]
C ₉ H ₉ N	skatole (c)	-1170.2	+16.3	[45, 46]
C ₉ H ₁₀ N ₂	dipyrrolymethane (c)	-1219.4	+31.4	[452]
C ₉ H ₁₅ N	phyllopyrrole (c) (2,4,5-trimethyl-3-ethyl pyrrole)	-1338.4	-20.4	[453]
C ₁₀ H ₈ N ₂ O ₂	4-phenyl uracil (c)	-1132.1	-81.7	[152]
C ₁₀ H ₉ N	<i>N</i> -phenylpyrrole (c)	-1286.0	+38.1	[452, 462]
C ₁₀ H ₉ N	α-phenylpyrrole (c)	-1282.4	+34.5	[452]
C ₁₀ H ₉ N	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 ₈ N ₂	phenazine (c)	-1458.3	+56.4	[6, 568]
C ₁₂ H ₉ N	carbazole (c)	-1466.3	+30.3	[45, 46, 526]
C ₁₂ H ₁₄ N ₄ O ₆	desoxyamalic acid (c)	-1321.1	-285.7	[294]
C ₁₂ H ₁₄ N ₄ O ₈	amalic acid (c)	-1239.8	-367.0	[294]
C ₁₃ H ₉ N	acridine (c)	-1574.9	+44.8	[6, 568]
C ₁₆ H ₁₀ N ₂ O ₂	indigotin (c)	-1814	-32	[5]
C ₁₆ H ₁₂ N ₂ O 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 ₂ O _{0.5}	amarine hemihydrate (c)	-2653	+29	[126, 131]
C ₂₄ H ₂₄ N ₂ O 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, ΔH_c° [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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₃₂ H ₃₆ N ₄ O 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 ₄ O ₂	γ-phyllporphyrin mono-methyl ester (c)	-4314.4	-87.3	[454]
C ₃₄ H ₃₄ N ₄ O ₄	protoporphyrin (c)	-4238.5	-120.6	[454]
C ₃₄ H ₃₆ N ₄ O ₃	phyllerythrin monomethyl ester (c)	-4344.2	-83.2	[454]
C ₃₄ H ₃₆ N ₄ O ₃	pyropheophorbide a mono-methyl ester (c)	-4342.6	-84.8	[454]

6.40. Porphyrins—Continued

Formula	Compound (State)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₃₄ H ₃₆ N ₄ O ₄	verdoporphyrin dimethyl ester (c)	-4284.1	-143.3	[454]
C ₃₄ H ₃₆ N ₄ O ₅	pheopurpurin 18 monomethyl ester (c)	-4196.6	-230.8	[454]
C ₃₄ H ₃₈ N ₄ O ₂	desoxyphyloerythrin monomethyl ester (c)	-4456.8	-38.9	[454]
C ₃₄ H ₃₈ N ₄ O ₄	rhodoporphyrin (XV) dimethyl ester (c)	-4373.5	-122.2	[454]
C ₃₄ H ₃₈ N ₄ O ₄	rhodoporphyrin (XXI) dimethyl ester (c)	-4371.8	-123.9	[454]
C ₃₅ H ₃₈ N ₄ O ₅	chloroporphyrin e ₅ dimethyl ester (c)	-4486.5	-103.3	[454]
C ₃₅ H ₄₀ N ₄ O ₄	chlorin e ₄ dimethyl ester (c)	-4513.2	-144.9	[454]
C ₃₅ H ₄₀ N ₄ O ₄	chloroporphyrin e ₄ dimethyl ester (c)	-4503.9	-154.2	[454]
C ₃₆ H ₃₆ N ₄ O ₆	methyl pheophorbide b (c)	-4414.8	-200.7	[454]
C ₃₆ H ₃₈ N ₄ O ₄	protoporphyrin dimethyl ester (c)	-4561.7	-122.1	[454]
C ₃₆ H ₃₈ N ₄ O ₅	methyl pheophorbide a (c)	-4527.7	-156.1	[454]
C ₃₆ H ₃₈ N ₄ O ₅	phcoporphyrin a ₅ dimethyl ester (c)	-4519.5	-164.3	[454]
C ₃₆ H ₄₀ N ₄ O ₆	chlorin p ₆ trimethyl ester (c)	-4460.1	-292.0	[454]
C ₃₆ H ₄₂ N ₄ O 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 ₄ O ₇	dimethyl pheopurpurin 7 (c)	-4600.4	-245.8	[454]
C ₃₇ H ₄₂ N ₄ O ₆	chloroporphyrin e ₆ trimethyl ester (c)	-4684.2	-230.3	[454]
C ₃₇ H ₄₂ N ₄ O ₆	chlorin e ₆ trimethyl ester (c)	-4693.1	-221.4	[454]
C ₄₀ H ₄₆ N ₄ O ₈	coproporphyrin (I) tetramethyl ester (c)	-4985.0	-348.3	[454]
C ₄₈ H ₅₄ N ₄ O 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
CH ₄ S	methanethiol (liq)	-363.48	-11.08	[165]
C ₂ H ₄ S	thiacyclopropane (liq)	-481.02	+12.41	[502, 505]
C ₂ H ₆ S	ethanethiol (liq)	-519.39	-17.53	[41, 298]
C ₂ H ₆ S	2-thiapropane (liq)	-521.37	-15.55	[298]
C ₂ H ₆ S ₂	1,2-ethanedithiol (liq)	-667.97	-12.83	[282]
C ₂ H ₆ S ₂	2,3-dithiabutane (liq)	-665.98	-14.82	[157, 187]
C ₃ H ₆ S	thiacyclobutane (liq)	-636.90	+5.93	[190, 295, 502, 505]
C ₃ H ₈ S	1-propanethiol (liq)	-675.51	-23.78	[192]
C ₃ H ₈ S ₂	1,3-propanedithiol (liq)	-824.34	-18.83	[282]
C ₄ H ₄ S	thiophene (liq)	-675.95	+19.24	[157, 191, 295, 317, 504, 505, 553]
C ₄ H ₈ S	thiacyclopentane (liq)	-775.95	-17.39	[124, 190, 295, 502, 505]

6.41. Organic Sulfur Compounds—Continued

Formula	Compound (State)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₄ H ₁₀ S	1-butanethiol (liq)	-831.97	-29.69	[189]
C ₄ H ₁₀ S ₂	1,4-butanedithiol (liq)	-980.42	-25.11	[282]
C ₅ H ₆ S	2-methylthiophene (liq)	-829.83	+10.75	[350]
C ₅ H ₆ S	3-methylthiophene (liq)	-829.46	+10.38	[299]
C ₅ H ₁₀ S	thiacyclohexane (liq)	-930.38	-25.33	[295, 297, 502, 505]
C ₅ H ₁₂ S	1-pentanethiol (liq)	-988.30	-35.72	[41, 190, 295, 503, 505]
C ₆ H ₆ S	benzenethiol (liq)	-928.45	+15.32	[427]
C ₆ H ₁₄ S	1-hexanethiol (liq)	-1144.55	-41.84	[163]
C ₇ H ₈ S	benzyl mercaptan (liq)	-1086.0	+10.4	[272, 275]
C ₇ H ₈ S	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 H₂SO₄ · 115H₂O (liq) as the final state of sulfur in the combustion values cited above, and have taken $\Delta H_f^\circ[\text{H}_2\text{SO}_4 \cdot 115\text{H}_2\text{O}(\text{liq})] = -212.192 \text{ kcal mol}^{-1}$ 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 CH₂ increment in the liquid state.

6.42. Organic Sulfur Compounds Containing Nitrogen and/or Oxygen

Formula	Compound (State)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
CH ₄ N ₂ S	thiourea (c)	-353.43	-21.13	[20, 293, 504]
C ₂ H ₄ OS	thiolacetic acid (liq)	-416.22	-52.39	[504, 505]
C ₂ H ₇ NO ₃ S	2-aminoethane-1-sulfonic acid (c) (taurine)	-383.4	-187.7	[34]
C ₃ H ₄ N ₂ OS	thiohydantoin (c)	-503.2	-59.5	[294]
C ₃ H ₆ O ₂ S	β -thiolactic acid (liq)	-519.4	-111.6	[81, 197]
C ₃ H ₆ N ₂ O ₂ S	thiohydantoic acid (c)	-498.4	-132.6	[294]
C ₃ H ₇ NO ₂ S	L-cysteine (c)	-540.5	-124.6	[20, 81, 197, 501]
C ₄ H ₂ N ₂ S	4-cyanothiazole (c)	-641.03	+52.63	[284]
C ₄ H ₅ NS	4-methylthiazole (liq)	-707.18	+16.31	[284]
C ₅ H ₁₁ NO ₂ S	L-methionine (c)	-809.5	-180.4	[535]
C ₆ H ₁₀ O ₄ S ₂	β, β' -dithiodilactic acid (liq)	-962.7	-230.9	[81, 197]
C ₆ H ₁₂ N ₂ S ₃	tetramethylthiuram monosulfide (c)	-1417.43	+11.60	[164]
C ₆ H ₁₂ N ₂ S ₄	tetramethylthiuramdisulfide(c)	-1559.64	+9.94	[164]
C ₆ H ₁₂ N ₂ O ₄ S ₂	L-cystine (c)	-1016.3	-245.7	[20, 81, 144, 197, 501]

We have used H₂SO₄ · 115H₂O(liq) as the final state for the sulfur in the combustion values cited above, and have taken $\Delta H_f^\circ[\text{H}_2\text{SO}_4 \cdot 115\text{H}_2\text{O}(\text{liq})] = -212.192 \text{ kcal mol}^{-1}$ 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)	$\Delta H_c^\circ 298 \text{ K}$ kcal mol ⁻¹	$\Delta H_f^\circ 298 \text{ K}$ kcal mol ⁻¹	Reference
C ₃ H ₉ P	trimethylphosphine (liq)	-763	-30	[258]
C ₆ H ₁₅ O ₄ P	triethyl phosphate (liq)	-983	-297	[25, 328]
C ₉ H ₂₁ O ₄ P	tri- <i>n</i> -propyl phosphate (liq)	-1452	-315	[415]
C ₁₂ H ₂₇ OP	tri- <i>n</i> -butyl phosphine oxide (c)	-2143	-110	[451]
C ₁₂ H ₂₇ O ₂ P	<i>n</i> -butyl ester of di- <i>n</i> -butyl- phosphinic acid (liq)	-2071	-183	[451]
C ₁₂ H ₂₇ O ₄ P	tri- <i>n</i> -butyl phosphate (liq)	-1906 (-1921)	-348 (-333)	[328, 451]
C ₁₂ H ₂₇ O ₄ P	triisobutyl phosphate (liq)	-1908	-346	[328]
C ₁₈ H ₁₅ O ₄ P	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 H₃PO₄(c) appears as the final standard

state of phosphorus, and have used $\Delta H_f^\circ[\text{H}_3\text{PO}_4(\text{c})] = -305.7 \text{ kcal mol}^{-1}$. 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 CH₂(liq) increment.

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

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8. Compound Index

A

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acetaldehyde, 232
 acetamide, 246
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 1-acetamido-2-nitroguanidine, 247
 5-acetamidotetrazole, 252
 acetanilide, 246
 acetic acid, 233
 acetic anhydride, 238
 acetone, see propanone
 acetone glyceraldehyde, 232

Empirical formula, WLN*

C₂H₄O, VH1
 C₂H₅NO, ZV1
 C₃H₉N₅O₄, MUYZMMV1 & H-N-O3
 C₃H₇N₅O₃, WNNUYZMMV1
 C₃H₅N₅O, T5MNNNJ EMV1
 C₃H₉NO, 1VMR
 C₂H₄O₂, QV1
 C₄H₆O₃, 1VOV1
 C₆H₁₀O₃, T5O COTJ B B DVH

* (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
acetone glycerol, 231	C ₆ H ₁₂ O ₃ , T50 COTJ B B DIQ
acetophenone, 233	C ₈ H ₈ O, IVR
acetylene, 226	C ₂ H ₂ , IUUI
cis-aconitic acid, 237	C ₆ H ₆ O ₆ , QV1YVQU1VQ -T
trans-aconitic acid, 237	C ₆ H ₆ O ₆ , QV1YVQU1VQ -C
acridine, 254	C ₁₃ H ₉ N, T C666 BNJ
acrylic acid, 235	C ₃ H ₄ O ₂ , QV1U1
adenine, 253	C ₅ H ₅ N ₅ , T56 BM DN FN HNJ IZ
adipic acid, 236	C ₆ H ₁₀ O ₄ , QV4VQ
aetioporphyrin (I), 255	C ₃₂ H ₃₈ N ₄ , T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-NJ E2 F J2 K O2 P T2 U
aetioporphyrin (II), 255	C ₃₂ H ₃₈ N ₄ , T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-NJ E2 F J K2 O2 P T U2
DL-alanine, 247	C ₃ H ₇ NO ₂ , ZYVQ
L-alanine, 247	C ₃ H ₇ NO ₂ , ZYVQ -B
alanine anhydride, 250	C ₆ H ₁₀ N ₂ O ₂ , T6MV DMVTJ C F
DL-alanylglycine, 250	C ₅ H ₁₀ N ₂ O ₃ , ZYVM1VQ
alanylphenylalanine, 251	C ₁₂ H ₁₆ N ₂ O ₃ , ZY&VMYVQ1R
alanylphenylalanine anhydride, 250	C ₁₂ H ₁₄ N ₂ O ₂ , T6MV DMVTJ C F1R
allantoin, 252	C ₄ H ₆ N ₄ O ₃ , T5MVMV EHJ EMVZ
allomucic acid, 236	C ₆ H ₁₀ O ₈ , QVYQYQ 2 -AAAA
alloxan monohydrate, 252	C ₄ H ₄ N ₂ O ₅ , T6MVMVVVJ &QH
alloxantin dihydrate, 254	C ₈ H ₁₀ N ₄ O ₁₀ , T6MVMV FHJ FQ F- 2 &QH &QH
1-allyl-5-allylaminotetrazole, 254	C ₇ H ₁₁ N ₅ , T5NNNNJ A2U1 EM2U1
1-allyl-5-aminotetrazole, 252	C ₄ H ₇ N ₅ , T5NNNNJ A2U1 EZ
2-allyl-5-aminotetrazole, 252	C ₄ H ₇ N ₅ , T5NNNNJ B2U1 EZ
amalic acid, 254	C ₁₂ H ₁₄ N ₂ O ₈ , T6VNVNV FHJ B D FQ F- 2
amarine, 254	C ₂₁ H ₁₈ N ₂ , T5M CN BUTJ BR& DR& ER
amarine hemihydrate, 254	C ₂₁ H ₁₉ N ₂ O _{0.5} , T5M CN BUTJ BR& DR& ER &/QH1/2
4-amino-3-azido-5-ethyl-s-triazole, 252	C ₄ H ₇ N ₇ , T5NN DNJ CNNN DZ E2
4-amino-3-azido-5-methyl-s-triazole, 252	C ₅ H ₈ N ₇ , T5NN DNJ CNNN DZ E
4-amino-3-azido-5-phenyl-s-triazole, 254	C ₈ H ₇ N ₇ , T5NN DNJ CNNN DZ ER
4-amino-3-azido-s-triazole, 251	C ₂ H ₃ N ₇ , T5NN DNJ CNNN DZ
5-aminobarbituric acid, see uramil	
m-aminobenzoic acid, 249	C ₇ H ₇ NO ₂ , ZR CVQ
o-aminobenzoic acid, 249	C ₇ H ₇ NO ₂ , ZR BVQ
p-aminobenzoic acid, 249	C ₇ H ₇ NO ₂ , ZR DVQ
γ-aminobutyric acid, 248	C ₄ H ₉ NO ₂ , Z3VQ
α-aminocaproic acid, 248	C ₆ H ₁₃ NO ₂ , ZY4&VQ
γ-aminocaproic acid, 248	C ₆ H ₁₃ NO ₂ , ZY2&2VQ
δ-aminocaproic acid, 248	C ₆ H ₁₃ NO ₂ , ZY3VQ
ε-aminocaproic acid, 248	C ₆ H ₁₃ NO ₂ , Z5VQ
ζ-aminobenanthylic acid, 248	C ₇ H ₁₅ NO ₂ , Z6VQ
2-aminoethane-1-sulfonic acid, 257	C ₂ H ₇ NO ₃ S Z2SWO
3-amino-5-methyl-1,2,4-triazole nitrate, 252	C ₃ H ₇ N ₅ O ₃ , T5MN DNJ CZ E & H-N-O3
ω-aminopelargonic acid, 248	C ₉ H ₁₉ NO ₂ , Z8VQ
5-aminotetrazole, 251	CH ₃ N ₅ , T5MNNNJ EZ
5-aminotetrazole nitrate, 251	CH ₃ N ₅ O ₃ , T5MNNNJ EZ & H-N-O3
3-amino-1,2,4-triazole, 251	C ₂ H ₄ N ₄ , T5MN DNJ CZ
3-amino-1,2,4-triazole nitrate, 251	C ₃ H ₅ N ₅ O ₃ , T5MN DNJ CZ & H-N-O3
δ-aminovaleric acid, 248	C ₅ H ₁₁ NO ₂ , Z4VQ
amygdalin, 243	C ₂₀ H ₂₇ NO ₁₁ , T60TJ BOYR&CN CQ DQ EQ F1O- BT60TJ CQ DQ EQ F1Q -A&CE -B&BDF -A&CE -B&BDF
n-amyl alcohol, see 1-pentanol	
5α-androstane, 240	C ₁₉ H ₃₂ , L E5 B666TJ A E -A&BIM -B&AEIJ
5α-androstane-3,17-dione, 240	C ₁₉ H ₂₈ O ₂ , L E5 B666 FV OVTJ A E -A&BIM -B&AEJ
5α-androstane-3α-ol-17-one, 240	C ₁₉ H ₃₀ O ₂ , L E5 B666 FVTJ A E OQ -A&BIMO -B&AEJ
5α-androstane-3β-ol-17-one, 240	C ₁₉ H ₃₀ O ₂ , L E5 B666 FVTJ A E OQ -A&BIM -B&AEJO
5α-androstane-3-one-17β-ol, 240	C ₁₉ H ₃₀ O ₂ , L E5 B666 OVTJ A E FQ -A&BIM -B&AEFJ
Δ ₄ -androstene-3,17-dione, 240	C ₁₉ H ₂₆ O ₂ , L E5 B666 FV OV MUTJ A E -A&BI -B&AEJ
Δ ₄ -androstene-3-one-17β-ol, 240	C ₁₉ H ₂₈ O ₂ , L E5 B666 OV MUTJ A E FQ -A&BI -B&AEJ
Δ ₅ -androstene-3β-ol-17-one, 240	C ₁₉ H ₂₈ O ₂ , L E5 B666 FV LUTJ A E OQ -A&BI -B&AEJO
androsterone, see 5α-androstane-3α-ol-17-one	
angelic acid, 235	C ₅ H ₈ O ₂ , QVYU2 -C
1,6-anhydroglucopyranoside, see levoglucosan	
1,2-anhydroglucose-3,5,6-triacetate, 242	
aniline, 246	C ₁₂ H ₁₈ O ₈ , T30TJ BYOV1&YQYOV1&1OV1 -B&B -BAA
aniline nitrate, 246	C ₆ H ₇ N, ZR
animal fat, 277	C ₆ H ₈ N ₂ O ₃ , ZR & H-N-O3
anisine, 254	
anisoyl glycine, 249	C ₂₄ H ₂₄ N ₂ O ₃ , T5M CN BUTJ B- D- E-/R DO1 3
anthracene, 227	C ₁₀ H ₁₁ NO ₄ , QV1MVR DO1
β-D-arabinose, 242	C ₁₄ H ₁₀ , L C666J
β-L-arabinose, 242	C ₅ H ₁₀ O ₅ , T60TJ BQ CQ DQ EQ -A&DE -B&BC
L-arabitol, 231	C ₅ H ₁₀ O ₅ , T60TJ BQ CQ DQ EQ -A&C -B&BDE
D-arabonic acid-γ-lactone, 241	C ₅ H ₁₂ O ₅ , Q1YQYQYQ1Q -BAA
arachidic acid, 234	C ₅ H ₈ O ₅ , T50VTJ CQ DQ E1Q -A&D -B&CE
L-arginine, 248	C ₂₀ H ₄₀ O ₂ , QV19
L-ascorbic acid, 241	C ₆ H ₁₄ N ₄ O ₂ , QVYZ3MYZUM -B
L-asparagine, 248	C ₆ H ₈ O ₈ , T50V EHJ CQ DQ EYQ1Q -A&E -A
L-asparagine monohydrate, 248	C ₈ H ₈ N ₂ O ₃ , ZV1YZVQ -A
L-aspartic acid, 248	C ₄ H ₁₀ N ₂ O ₄ , ZV1YZVQ -A &QH
3-azido-5-ethyl-s-triazole, 252	C ₄ H ₇ NO ₄ , QVYZ1VQ -B
	C ₄ H ₈ N ₆ , T5NN DMJ CNNN E2

Compound name, page	Empirical formula, WLN
3-azido-5-methyl-s-triazole, 252	C ₃ H ₄ N ₆ , T5NN DMJ CNNN E
3-azido-5-phenyl-s-triazole, 254	C ₈ H ₆ N ₆ , T5NN DMJ CNNN ER
3-azido-s-triazole, 251	C ₂ H ₂ N ₆ , T5NN DMJ CNNN
azodicarbamide, 247	C ₂ H ₄ N ₄ O ₂ , ZVNUNVZ
B	
barbituric acid, 252	C ₄ H ₄ N ₂ O ₃ , T6VMVMV FHJ
behenic acid, 234	C ₂₂ H ₄₄ O ₂ , QV21
benzaldehyde, 232	C ₇ H ₆ O, VHR
benzalhippuric acid, 249	C ₁₆ H ₁₃ NO ₃ , RVMYVQUIR
benzalhippuric acid azlactone, 249	C ₁₆ H ₁₁ NO ₂ , T5NYVOJ BUIR& ER
benzamide, 246	C ₇ H ₇ NO, ZVR
benzanilide, 247	C ₁₃ H ₁₂ NO, RVMR
1,2-benzanthracene, 228	C ₁₈ H ₁₂ , L D6 B666J
benzene, 227	C ₆ H ₆ , R
benzenethiol, 257	C ₆ H ₆ S, SHR
benzoic acid, 237	C ₇ H ₆ O ₂ , QVR
benzophenone, 233	C ₁₃ H ₁₀ O, RVR
benzotriazole, 253	C ₆ H ₅ N ₃ , T56 BMNNJ
DL-benzoylalanine, 249	C ₁₀ H ₁₁ NO ₃ , QVYMVR
benzoylphenylalanine, 249	C ₁₆ H ₁₅ NO ₃ , QVY1R&MVR
benzoyl sarcosine, 249	C ₁₀ H ₁₁ NO ₃ , QV1N1&VR
3,4-benzphenanthrene, 228	C ₁₈ H ₁₂ , L C6 B666J
benzyl mercaptan, 257	C ₇ H ₈ S, SH1R
blood fibrin, 277	
brassicic acid, 235	C ₂₂ H ₄₂ O ₂ , QV12U9 -T
brucine, 251	C ₂₃ H ₂₆ N ₂ O ₄ , T6 G656 B7 C6 E5 D 5ABCEF A& FX MNV QO VN SU AHT&&ITTTJ IO1 JO1
1-butanal, see <i>n</i> -butyraldehyde	
<i>n</i> -butane, 226	C ₄ H ₁₀ , 4H
1,2-butanediamine, 245	C ₄ H ₁₂ N ₂ , ZY2&1Z
2,3-butanedione, 233	C ₄ H ₆ O ₂ , 1VV1
1,4-butanedithiol, 257	C ₄ H ₁₀ S ₂ , SH4SH
1-butanethiol, 257	C ₄ H ₁₀ S, SH4
butanoic acid, see butyric acid	
1-butanol, 229	C ₄ H ₁₀ O, Q4
2-butanol, 229	C ₄ H ₁₀ O, QY2
butanone, 232	C ₄ H ₈ O, 2V1
<i>n</i> -butyl alcohol, see 1-butanol	
sec.-butyl alcohol, see 2-butanol	
tert.-butyl alcohol, see 2-methyl-2-propanol	
<i>n</i> -butylamine, 245	C ₄ H ₁₁ N, Z4
sec.-butylamine, 245	C ₄ H ₁₁ N, ZY2
tert.-butylamine, 245	C ₄ H ₁₁ N, ZX
<i>n</i> -butyl di- <i>n</i> -butyl phosphinate, see <i>n</i> -butyl ester of di- <i>n</i> -butyl phosphinic acid	
<i>n</i> -butyl ester of di- <i>n</i> -butylphosphinic acid, 258	C ₁₂ H ₂₇ O ₂ P, OP4&4&O4
butter, 277	
<i>n</i> -butyraldehyde, 232	C ₄ H ₈ O, VH3
<i>n</i> -butyramide, 246	C ₄ H ₉ NO, ZV3
butyric acid, 233	C ₄ H ₈ O ₂ , QV3
C	
caffeine, 254	C ₈ H ₁₀ N ₄ O ₂ , T56 BN DN FNVNVJ B F H
calcium 1-glycerol phosphate, 277	
calcium hexose phosphate, 277	
capric acid, 233	C ₁₀ H ₂₀ O ₂ , QV9
caproic acid, 233	C ₆ H ₁₂ O ₂ , QV5
ε-caprolactam, 253	C ₆ H ₁₁ NO, T7MVTJ
caprylic acid, 233	C ₈ H ₁₆ O ₂ , QV7
carbazole, 254	C ₁₂ H ₉ N, T B656 HMJ
α-carbethoxyglycylglycine ethyl ester, 250	C ₉ H ₁₆ N ₂ O ₅ , 2OV1M1V02
β-carbethoxyglycylglycine ethyl ester, 250	C ₉ H ₁₆ N ₂ O ₅ , 2OV1M 2V
cellobiose, 243	C ₁₂ H ₂₂ O ₁₁ , T6OTJ BQ CQ DQ FIQ EO- BT6OTJ CQ DQ EQ FIQ -A&CE -B&BDF -A&CE -B&BDF
cellobiose octaacetate, 243	C ₂₈ H ₃₈ O ₁₉ , T6OTJ BOV1 COV1, DOV1 FIOV1 EO- BT6OTJ COV1 DOV1 EOVI FIOV1 -A&CE -B&BDF -A&CE -B&BDF
cellulose, 277	
cellulose hexaacetate, 277	
chlorin <i>e</i> ₄ dimethyl ester, 256	C ₃₅ H ₄₀ N ₄ O ₄ , T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-N&&&&TJ C EVO1 F J2 K O1U1 P T U2VO1
chlorin <i>e</i> ₆ trimethyl ester, 256	C ₃₇ H ₄₂ N ₄ O ₆ , T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-N&&&&TJ C1VO1 EVO1 F J2 K O1U1 P T U2VO1
chlorin <i>p</i> ₆ trimethyl ester, 256	C ₃₆ H ₄₀ N ₄ O ₆ , T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-N&&&&TJ CVO1 EVO1 F J2 K O1U1 P T U2VO1

Compound name, page	Empirical formula, WLN
chloroporphyrin e_4 dimethyl ester, 256	$C_{35}H_{40}N_4O_4$, T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-NJ C EVO1 F J2 K O2 P T U2VO1
chloroporphyrin e_5 dimethyl ester, 256	$C_{35}H_{38}N_4O_5$, T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-NJ CVH EVO1 F J2 K O2 P T U2VO1
chloroporphyrin e_6 trimethyl ester, 256	$C_{37}H_{42}N_4O_6$, T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-NJ C1VO1 EVO1 F J2 K O2 P T U2VO1
5 β -cholan-24-oic acid-3 α ,7 α ,12 α -triol monohydrate, 241	$C_{24}H_{42}O_8$, L E5 B666TJ A DQ E FY2VQ KQ OQ -A&BDIKO -B&AEFJM &QH
Δ_5 -cholestene-3 β -ol, 241	$C_{27}H_{46}O$, L E5 B666 LUTJ A E FY&3Y OQ -A&BI -B&AEFO
Δ_5 -cholestene-3 β -methyl ether, 241	$C_{28}H_{48}O$, L E5 B666 LUTJ A E FY&3Y OO1 -A&BI -B&AEFO
cholesterol, see Δ_5 -cholestene-3 β -ol	
cholesterol methyl ether, see Δ_5 -cholestene-3 β -methyl ether	
cholic acid monohydrate, see 5 β -cholan-24-oic acid-3 α ,7 α ,12 α -triol monohydrate	
chrysene, 228	$C_{18}H_{12}$, I E6 B666J
cinchonamine, 251	$C_{19}H_{24}N_2O$, T66 A B CNTJ A1U1 D- CT56 BMJ D2Q -A&DF -B&A
cinchonamine nitrate, 251	$C_{19}H_{25}N_3O_4$, T66 A B CNTJ A1U1 D- CT56 BMJ D2Q -A&DF -B&A & H-N-O3
cinchonidine, 251	$C_{10}H_{22}N_6O$, T66 BNJ EYQ- DT66 A B CNTJ A1U1 -A&F -B&AD
cinchonine, 251	$C_{19}H_{22}N_2O$, T66 BNJ EYQ- DT66 A B CNTJ A1U1 -A&DF -B&A
citraconic acid, 237	$C_5H_6O_4$, QVYU1VQ -C
citric acid (anhydrous), 236	$C_6H_8O_7$, QVIXQVQ1VQ
citric acid monohydrate, 236	$C_6H_{10}O_8$, QVIXQVQ1VQ &QH
codeine monohydrate, 251	$C_{18}H_{23}NO$, T B6566 B6/CO 4ABBC R BX HO PN DU GHT&TTJ FQ JO1 P -A&FO -B&BCG &QH
conglutin, 277	$C_6H_{17}N$, T6MTJ B3
coniine, 251	$C_{40}H_{46}N_4O_8$, T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-NJ E2VO1 F J2VO1 K O2VO1 P T2VO1 U
coproporphyrin (I) tetramethyl ester, 256	
cortexone, see Δ_4 -pregnene-3,20-dione-21-ol	
cortisol, see Δ_4 -pregnene-3,20-dione-11 β ,17 α ,21-triol	
cortisone, see Δ_4 -pregnene-3,11,20-trione-17 α ,21-diol	
creatine, 247	$C_4H_9N_3O_2$, QVIN1&YZUM
creatine hydrate, 247	$C_4H_{11}N_3O_3$, QVIN1&YZUM &QH
creatinine, 252	$C_4H_7N_3O$, T5NYMV EHJ A BUM
<i>m</i> -cresol, 230	C_7H_8O , QR C
<i>o</i> -cresol, 230	C_7H_8O , QR B
<i>p</i> -cresol, 230	C_7H_8O , QR D
<i>cis</i> -crotonic acid, 235	$C_4H_6O_2$, QV1U2 -C
<i>trans</i> -crotonic acid, 235	$C_4H_6O_2$, QV1U2 -T
3-cyanopyridine, 253	$C_6H_4N_2$, T6NJ CCN
5-cyanotetrazole, 251	C_2HN_5 , T5MNNNJ ECN
4-cyanothiazole, 257	$C_4H_2N_2S$, T5N CSJ ECN
cyclobutane, 226	C_4H_8 , L4TJ
3:5-cyclocholestan-6 β -yl methyl ether, 241	$C_{28}H_{48}O$, L E5 D6653 1A Q AXTJ BO1 HY&3Y I M -A&ABDHIM -B&ELP
cycloheptane, 227	C_7H_{14} , L7TJ
cyclohexane, 226	C_6H_{12} , L6TJ
cyclooctane, 227	C_8H_{16} , L8TJ
cyclopentane, 226	C_5H_{10} , L5TJ
cyclopropane, 226	C_3H_6 , L3TJ
L-cysteine, 247	$C_3H_7NO_2S$, SH1YZVQ -A
L-cystine, 248	$C_6H_{12}N_2O_4S_2$, QVYZIS 2 -BA
1,10-decanediol, 231	
decanoic acid, see capric acid	
<i>trans</i> -dehydroandrosterone, see Δ_5 -androstane-3 β -ol-17-one	
dehydro- β -campholenolactone (dextrorotatory), 241	
dehydro- β -campholenolactone (inactive), 241	
desoxyamalic acid, 254	
desoxycorticosterone, see Δ_4 -pregnene-3,20-dione-21-ol	
desoxyphyloerythrin monomethyl ester, 256	
dextran, 277	
diacetamide, 246	
1,2,5,6-diacetone mannitol, 231	
diacetyl, see 2,3-butanedione	
diacetyl xylan, 277	
5-diallylamino-tetrazole, 254	
dialuric acid, 252	
	$C_{34}H_{38}N_4O_2$, T-T55 BN HY&TJ D HU- AT5MYJ D E2VO1 CU1- ET5NYJ C2 D BU1- BT5MJ C D2 E1U- C-16-J
	$C_4H_7NO_2$, 1VMV1
	$C_{12}H_{22}O_6$, T5O COTJ B B DYQ 2 -A&D -AB -B&D
	$C_7H_{11}N_5$, T5MNNNJ EN2U1&2U1
	$C_4H_4N_2O_4$, T6VMVMV FHJ FQ

D

 $C_{10}H_{22}O_2$, Q10Q

$C_{10}H_{16}O_2$, T55 BOVTJ A G G -D
 $C_{10}H_{16}O_2$, T55 BOVTJ A G G
 $C_{12}H_{14}N_4O_6$, T6VNVNV FHJ B D F- 2

$C_{34}H_{38}N_4O_2$, T-T55 BN HY&TJ D HU-
AT5MYJ D E2VO1 CU1- ET5NYJ C2 D
BU1- BT5MJ C D2 E1U- C-16-J

$C_4H_7NO_2$, 1VMV1
 $C_{12}H_{22}O_6$, T5O COTJ B B DYQ 2 -A&D -AB -B&D

$C_7H_{11}N_5$, T5MNNNJ EN2U1&2U1
 $C_4H_4N_2O_4$, T6VMVMV FHJ FQ

Compound name, page	Empirical formula, WLN
<i>sym</i> -diaminoguanidine nitrate, 247	CH ₈ N ₆ O ₃ , ZMYUM&MZ & H-N-O3
2,6-diaminopyridine, 253	C ₅ H ₇ N ₃ , T6NJ BZ FZ
diamylose, 244	C ₂₄ H ₄₀ O ₂₀ , T6OTJ BQ CQ DQ F1Q EO-/
	BT6OTJ CQ DQ F1Q EO-/ 2 BT6OTJ CQ
	DQ EQ F1Q -A&CE -B&DF /-A&BCE
	-B&DF/ 3
diethylamine, 245	C ₄ H ₁₁ N, 2M2
diethylamine nitrate, 245	C ₄ H ₁₂ N ₂ O ₃ , 2M2 & H-N-O3
2,2'-diethyl-5,5'-azotetrazole, 253	C ₈ H ₁₀ N ₁₀ , T5NNNNJ B2 EN 2U
diethylbarbituric acid, 254	C ₈ H ₁₂ N ₂ O ₃ , T6VMVMV FHJ F2 F2
diethylenetriaminepentaacetic acid, 248	C ₁₄ H ₂₃ N ₃ O ₁₀ , QV1N1VQ2 2N1VQ
diethyl ether, 231	C ₄ H ₁₀ O, 2O2
diethyl ketone, see 3-pentanone	
diglycolamidic acid, 248	C ₄ H ₇ NO ₄ , QV1M1VQ
diglycylglycine, 250	C ₆ H ₁₁ N ₂ O ₄ , Z1VM1VM1VQ
dihydropyran, 4H, 244	C ₅ H ₈ O, T6O BUTJ
13,14-dihydroxybehenic acid, 235	C ₂₂ H ₄₄ O ₄ , QY8&YQ11VQ
1,2-dihydroxybenzene, see pyrocatechol	
1,3-dihydroxybenzene, see resorcinol	
1,4-dihydroxybenzene, see hydroquinone	
diketene, see β -methylene- β -propiolactone	
1,2-dimethoxyethane, 231	C ₄ H ₁₀ O ₂ , 1O2O1
<i>cis</i> - α,β -dimethylacrylic acid, see tiglic acid	
<i>trans</i> - α,β -dimethylacrylic acid, see angelic acid	
dimethyl adipate, 239	C ₈ H ₁₄ O ₄ , 1OV4VO1
dimethylamine, 245	C ₂ H ₇ N, 1M1
dimethylamine nitrate, 245	C ₂ H ₈ N ₂ O ₃ , 1M1 & H-N-O3
5-dimethylaminotetrazole, 252	C ₄ H ₇ N ₅ , T5MNNNJ EN1&1
<i>N,N</i> -dimethylaniline, 246	C ₈ H ₁₁ N, 1N1&R
<i>cis</i> ,1,1'-dimethyl-5,5'-azotetrazole, 252	C ₄ H ₆ N ₁₀ , T5NNNNJ A EN 2U -C
<i>trans</i> ,1,1'-dimethyl-5,5'-azotetrazole, 252	C ₄ H ₆ N ₁₀ , T5NNNNJ A EN 2U -T
2,2'-dimethyl-5,5'-azotetrazole, 252	C ₄ H ₆ N ₁₀ , T5NNNNJ B EN 2U
dimethyl ether, 231	C ₂ H ₆ O, 1O1
<i>N,N</i> -dimethylformamide, 246	C ₃ H ₇ NO, VHN1&1
dimethyl fumarate, 239	C ₆ H ₈ O ₄ , 1OV1U1VO1 -T
dimethyl glutarate, 239	C ₇ H ₁₂ O ₄ , 1OV3VO1
5,5-dimethyl hydantoin, 253	C ₅ H ₈ N ₂ O ₂ , T5MVMV EHJ E E
1,3-dimethyl-5-iminotetrazole nitrate, 252	C ₃ H ₈ N ₆ O ₃ , T5NNNNYJ A C EUM & H-N-O3
dimethyl maleate, 239	C ₆ H ₈ O ₄ , 1OV1U1VO1 -C
dimethyl malonate, 239	C ₆ H ₈ O ₄ , 1OV1VO1
dimethyl oxalate, 239	C ₄ H ₆ O ₄ , 1OVVO1
dimethyl parabanic acid, 253	C ₃ H ₆ N ₂ O ₃ , T5VNVNVJ B D
dimethyl pheopurpurin 7, 256	C ₃₇ H ₄₀ N ₄ O ₇ , T D5 I5 N5-16-5 A D- I-
	N- AM D-N I-M N-N&&&TJ CVVO1 EVO1
	F J2 K O1U1 P T U2VO1
dimethyl <i>m</i> -phthalate, 239	C ₁₀ H ₁₀ O ₄ , 1OVR CVO1
dimethyl <i>o</i> -phthalate, 239	C ₁₀ H ₁₀ O ₄ , 1OVR BVO1
dimethyl <i>p</i> -phthalate, 239	C ₁₀ H ₁₀ O ₄ , 1OVR DVO1
2,3-dimethylpyridine, 253	C ₇ H ₉ N, T6NJ B C
2,4-dimethylpyridine, 253	C ₇ H ₉ N, T6NJ B D
2,5-dimethylpyridine, 253	C ₇ H ₉ N, T6NJ B E
2,6-dimethylpyridine, 253	C ₇ H ₉ N, T6NJ B F
3,4-dimethylpyridine, 253	C ₇ H ₉ N, T6NJ C D
3,5-dimethylpyridine, 253	C ₇ H ₉ N, T6NJ C E
dimethyl succinate, 239	C ₆ H ₁₀ O ₄ , 1OV2VO1
1,5-dimethyl tetrazole, 252	C ₃ H ₆ N ₄ , T5NNNNJ A E
1,4-dimethyl-5-tetrazolone, 252	C ₃ H ₆ N ₄ O, T5NNNNVJ A D
1,3-dioxane, 244	C ₄ H ₈ O ₂ , T6O COTJ
1,4-dioxane, 244	C ₄ H ₈ O ₂ , T6O DOTJ
dioxindole, 254	C ₈ H ₇ NO ₂ , T56 BMV DHJ DQ
dipentaerythritol, 231	C ₁₀ H ₂₂ O ₇ , Q1X1Q1Q1 20
diphenyl disulfide, 257	C ₁₂ H ₁₀ S ₂ , RSSR
diphenyl sulfide, 257	C ₁₂ H ₁₀ S, RSR
dipotassium glucose-1-phosphate, 277	
di- α -pyrrol ketone, 254	C ₆ H ₈ N ₂ O, T5MJ B- 2V
dipyrrolymethane, 254	C ₃ H ₁₀ N ₂ , T5MJ B- 21
disodium glycerol-1-phosphate, 277	
disodium glycerol-2-phosphate, 277	
1,2-di-(5-tetrazolyl)ethane, 252	C ₄ H ₆ N ₈ , T5MNNNJ E- 22
2,3-dithiabutane, 256	C ₄ H ₆ S ₂ , 1SS1
β,β' -dithiodilactic acid, 257	C ₆ H ₁₀ O ₄ S ₂ , QVY&S 2
docosanoic acid, see behenic acid	
dodecanoic acid, see lauric acid	
dulcitol, 231	C ₆ H ₁₄ O ₆ , Q1YQYQ 2 -ABBA
egg albumin, 277	
eicosanoic acid, see arachidic acid	
elaidic acid, 235	C ₁₈ H ₃₄ O ₂ , QV8U9 -T
enanthalic acid, 233	C ₇ H ₁₄ O ₂ , QV6
ζ -enanthalactam, 254	C ₇ H ₁₃ NO, T8MVTJ
epiandrosterone, see 5 α -androstane-3 β -ol-17-one	
erucic acid, 235	C ₂₂ H ₄₂ O ₂ , QV12U9 -C

E

Compound name, page	Empirical formula, WLN
erythritol diacetal, 244	C ₈ H ₁₄ O ₄ , T5O COTJ B D- 2
erythritol diformal, 244	C ₆ H ₁₀ O ₄ , T5O COTJ D- 2
ethanal, see acetaldehyde	
ethane, 226	C ₂ H ₆ , 2H
1,2-ethanediol, 231	C ₂ H ₆ O ₂ , Q2Q
1,2-ethanedithiol, 256	C ₂ H ₆ S ₂ , SH2SH
ethanethiol, 256	C ₂ H ₆ S, SH2
ethanoic acid, see acetic acid	
ethanol, 229	C ₂ H ₆ O, Q2
ethyl alcohol, see ethanol	
ethylamine, 245	C ₂ H ₇ N, Z2
ethylamine nitrate, 245	C ₂ H ₈ N ₂ O ₃ , Z2 & H-N-O3
ethyl β-anilino-β-phenyl propionate, 249	C ₁₇ H ₁₉ NO ₂ , 2OV1YR&MR
ethyl carbamate, 246	C ₃ H ₇ NO ₂ , ZVO2
ethylene, 226	C ₂ H ₄ , 1U1
ethylene carbonate, 244	C ₃ H ₄ O ₃ , T5OVOTJ
ethylenediamine, 245	C ₂ H ₈ N ₂ , Z2Z
ethylenediamine dinitrate, 245	C ₂ H ₁₀ N ₄ O ₆ , Z2Z & H-N-O3*2
ethylenediaminetetraacetic acid, 248	C ₁₀ H ₁₆ N ₂ O ₈ , QV1N1VQ 22
ethylene glycol, see 1,2-ethanediol	
ethylenimine, 251	C ₂ H ₅ N, T3MTJ
ethyl glycylglycinate, 250	C ₆ H ₁₂ N ₂ O ₃ , Z1VM1VO2
2-ethylphenol, 230	C ₈ H ₁₀ O, QR B2
3-ethylphenol, 230	C ₈ H ₁₀ O, QR C2
4-ethylphenol, 230	C ₈ H ₁₀ O, QR D2
2-ethylpyridine, 253	C ₇ H ₉ N, T6NJ B2
F	
fluoranthene, 228	C ₁₆ H ₁₀ , L C6566 1A' PJ
formaldehyde, 232	CH ₂ O, VHH
formamide, 246	CH ₃ NO, ZVH
1-formamido-2-nitroguanidine, 247	C ₂ H ₅ N ₅ O ₃ , WNNUYZMMVH
formanilide, 246	C ₇ H ₇ NO, VHMR
formic acid, 233	CH ₂ O ₂ , VHQ
N-formyl-DL-leucine, 248	C ₇ H ₁₃ NO ₃ , VHMVQ1Y
formylurea, 247	C ₂ H ₄ N ₂ O ₂ , ZVMVH
β-D-fructose, 242	C ₆ H ₁₂ O ₆ , T6OTJ BQ B1Q CQ DQ EQ -A&DE -B&BC
D-fucose, 242	C ₆ H ₁₂ O ₆ , VHYQYQYQYQ -ABBA
fumaric acid, 237	C ₄ H ₄ O ₄ , QV1UIVQ -T
furane, 244	C ₄ H ₄ O, T5OJ
furfural, 244	C ₅ H ₄ O ₂ , T5OJ BVH
furfuryl alcohol, 244	C ₅ H ₆ O ₂ , T5OJ B1Q
2-furoic acid, 244	C ₅ H ₄ O ₃ , T5OJ BVQ
G	
D-galactonic acid, 235	C ₆ H ₁₂ O ₇ , QVYQYQYQYQ1Q -ABBA
D-galactonic acid-γ-lactone, 241	C ₆ H ₁₀ O ₆ , T5OVTJ CQ DQ EYQ1Q -A&C -B&DE -A
α-D-galactose, 242	C ₆ H ₁₂ O ₆ , T6OTJ BQ CQ DQ EQ F1Q -A&BC -B&DEF
galactose pentaacetate, 242	C ₁₆ H ₂₂ O ₁₁ , T6OTJ BOV1 COV1 DOV1 EOVI FIOV1 -A&C -B&DEF
gliadin, 277	C ₈ H ₈ O ₇ , T5OVTJ CQ DQ EYQVQ -A&CE -B&D -A
D-glucaric acid-1,4-lactone, 241	C ₆ H ₈ O ₇ , T5OVTJ CQ DQ EYQVQ -A&CD -B&E -A
D-glucaric acid-3,6-lactone, 241	C ₇ H ₁₂ O ₇ , T5OVTJ CQ DQ EYQYQ1Q -A&CD -B&E -AA
D-gluco-D-gulo-heptonic acid-γ-lactone, 241	C ₇ H ₁₆ O ₇ , Q1/YQ/ 51Q -AABAA
D-gluco-α-heptite, 231	
D-gluco-α-heptonic acid-γ-lactone, see D-gluco-D-gulo-heptonic acid-γ-lactone	
D-gluco-α-heptose, 242	C ₇ H ₁₄ O ₇ , VH/YQ/ 51Q -AABAA
D-gluconic acid, 235	C ₆ H ₁₂ O ₇ , QVYQYQYQYQ1Q -ABAA
D-gluconic acid-δ-lactone, 241	C ₆ H ₁₀ O ₆ , T6OVTJ CQ DQ EQ F1Q -A&CEF -B&D
D-gluco-α,α-octonic acid-γ-lactone, 241	C ₈ H ₁₄ O ₈ , T5OVTJ CQ DQ EYQYQYQ1Q -A&CDE -BAA
α-D-glucose, 242	C ₆ H ₁₂ O ₆ , T6OTJ BQ CQ DQ EQ F1Q -A&BCE -B&DF
β-D-glucose, 242	C ₆ H ₁₂ O ₆ , T6OTJ BQ CQ DQ EQ F1Q -A&CE -B&RDF
α-D-glucose hydrate, 242	C ₆ H ₁₄ O ₇ , T6OTJ BQ CQ DQ EQ F1Q -A&BCE -B&DF &QH
glucose pentaacetate, 242	C ₁₆ H ₂₂ O ₁₁ , T6OTJ BOV1 COV1 DOV1 EOVI FIOVI -A&CE -B&DF
L-glutamic acid, 248	C ₆ H ₉ NO ₄ , QVYZ2VQ -B
L-glutamine, 248	C ₅ H ₁₀ N ₂ O ₃ , ZV2YZVQ -A
glutaric acid, 236	C ₅ H ₈ O ₄ , QV3VQ
gluten, 277	
glutenin, 277	
glyceraldehyde, 232	C ₃ H ₆ O ₃ , VHYQ1Q
glycerol, see 1,2,3-propanetriol	
glyceryl-1-acetate, 239	C ₅ H ₁₀ O ₄ , Q1YQ1OV1
glyceryl-1-benzoate, 239	C ₁₀ H ₁₂ O ₄ , Q1YQ1OVR
glyceryl-2-benzoate, 240	C ₁₀ H ₁₂ O ₄ , Q1Y1QOVR
glyceryl-1-caprate, 240	C ₁₃ H ₂₆ O ₄ , Q1YQ1OV9
glyceryl-2-caprate, 240	C ₁₃ H ₂₆ O ₄ , Q1Y1QOV9
glyceryl-1,3-diacetate, 239	C ₇ H ₁₂ O ₅ , 1VO1YQ1OV1
glyceryl dibrassidate, 240	C ₄₇ H ₈₈ O ₅ , 9U12VO1 2YQ -TT
glyceryl dierucate, 240	C ₄₇ H ₈₈ O ₅ , 9U12VO1 2YQ -CC
glyceryl-1-laurate, 240	C ₁₅ H ₃₀ O ₄ , Q1YQ1OV11

Compound name, page	Empirical formula, WLN
glyceryl-2-laurate, 240	C ₁₅ H ₃₀ O ₄ , Q1Y1QOV11
glyceryl-1-myristate, 240	C ₁₇ H ₃₄ O ₄ , Q1YQ1OV13
glyceryl-2-myristate, 240	C ₁₇ H ₃₄ O ₄ , Q1Y1QOV13
glyceryl-1-palmitate, 240	C ₁₉ H ₃₈ O ₄ , Q1YQ1OV15
glyceryl-2-palmitate, 240	C ₁₉ H ₃₈ O ₄ , Q1Y1QOV15
glyceryl-1-stearate, 240	C ₂₁ H ₄₂ O ₄ , Q1YQ1OV17
glyceryl-2-stearate, 240	C ₂₁ H ₄₂ O ₄ , Q1Y1QOV17
glyceryl triacetate, 239	C ₉ H ₁₄ O ₆ , 1VO1 2YOV1
glyceryl tribenzoate, 240	C ₂₄ H ₂₀ O ₆ , RVO1 2YOV1
glyceryl tribenzoate, 240	C ₆₉ H ₁₂₈ O ₆ , 9U12VO 3/1Y1/ -TTT
glyceryl tributyrate, 240	C ₁₅ H ₂₆ O ₆ , 3VO1 2YOV3
glyceryl trierucate, 240	C ₆₉ H ₁₂₈ O ₆ , 9U12VO 3/1Y1/ -CCC
glyceryl trilaurate, 240	C ₃₈ H ₇₄ O ₆ , 11VO 3/1Y1/
glyceryl trimyristate, 240	C ₄₅ H ₈₆ O ₆ , 13VO 3/1Y1/
glycine, 247	C ₂ H ₅ NO ₂ , Z1VQ
glycine anhydride, 250	C ₄ H ₆ N ₂ O ₂ , T6MV DMVTJ
glycine nitrate, 247	C ₂ H ₆ N ₂ O ₅ , Z1VQ & H-N-O3
glycogen, 277	
glycol acetal, 244	C ₄ H ₈ O ₂ , T50 COTJ B
glycolic acid, 235	C ₂ H ₄ O ₃ , QV1Q
glycylalanylphenylalanine, 251	C ₁₁ H ₁₆ N ₂ O ₄ , Z1VMY&VMYVQ1R
glycylglycine, 250	C ₄ H ₈ N ₂ O ₃ , Z1VM1VQ
glycylglycine-N-carboxylic acid, 250	C ₅ H ₈ N ₂ O ₅ , QVM1VM1VQ
glycylphenylalanine, 250	C ₁₁ H ₁₄ N ₂ O ₃ , Z1VMYVQ1R
glycylphenylalanine anhydride, 250	C ₁₁ H ₁₂ N ₂ O ₂ , T6MV DMVTJ C1R
glycyltyrosyl anhydride, 250	C ₁₁ H ₁₂ N ₂ O ₃ , T6MV DMVTJ C1R DQ
glycylvaline, 250	C ₇ H ₁₄ N ₂ O ₃ , Z1VMYVQY
glycylvalyl anhydride, 250	C ₇ H ₁₂ N ₂ O ₂ , T6MV DMVTJ CY
glyoxal, 232	C ₂ H ₂ O ₂ , VHVH
glyoxylic acid, 235	C ₂ H ₄ O ₄ , VHVQ &QH
guanidine, 247	CH ₅ N ₃ , ZYZUM
guanidine carbonate, 247	C ₃ H ₁₂ N ₆ O ₃ , ZYZUM & 2 &QVQ
guanidine nitrate, 247	CH ₆ N ₄ O ₃ , ZYZUM & H-N-O3
guanine, 253	C ₅ H ₅ N ₅ O, T56 BN DM FN HNJ CZ IQ
5-guanylamino-tetrazole, 251	C ₂ H ₅ N ₇ , T5MNNNJ EMYZUM
guanyurea nitrate, 247	C ₂ H ₇ N ₅ O ₄ , ZVMYUM & H-N-O3
L-gulonic acid-γ-lactone, 241	C ₆ H ₁₀ O ₆ , T5OVTJ CQ DQ EYQ1Q -A&CD -B&E -A
H	
n-heptaldehyde, 232	C ₇ H ₁₄ O, VH6
1-heptanal, see n-heptaldehyde	
heptanoic acid, see enanthic acid	
hexadecanoic acid, see palmitic acid	
hexa-2-ene-1,6-dioic acid, 237	C ₆ H ₈ O ₄ , QV3U1VQ
hexa-3-ene-1,6-dioic acid, 237	C ₆ H ₈ O ₄ , QV2U2VQ
hexamethylene-1,6-diamine-adipic acid adduct, 248	C ₁₂ H ₂₆ N ₂ O ₄ , QV4VQ &Z6Z
hexamethylenetetramine, 253	C ₆ H ₁₂ N ₄ , T66 B6 A B- C 1B I BN DN FN HNTJ
hexamethylenetetramine dinitrate, 253	C ₆ H ₁₄ N ₆ O ₆ , T66 B6 A B- C 1B I BN DN FN HNTJ & H-N-O3*2
β-hexamyllose, 244	C ₄₈ H ₈₆ O ₄₀ , T6OTJ BQ CQ DQ F1Q EO-/ BT6OTJ CQ DQ F1Q EO-/ 6 BT6OTJ CQ DQ EQ F1Q -A&CE -B&BDF/ -A&BCE -B&DF/ 7
n-hexane, 226	C ₆ H ₁₄ , 6H
1-hexanethiol, 257	C ₆ H ₁₄ S, SH6
hexanoic acid, see caproic acid	
1-hexanol, 229	C ₆ H ₁₄ O, Q6
n-hexyl alcohol, see 1-hexanol	
hippuric acid, 249	C ₉ H ₉ NO ₃ , QV1MVR
hippurylglycine, 250	C ₁₁ H ₁₂ N ₂ O ₄ , QV1VM1MVR
human fat, 277	
hydantoic acid, 247	C ₃ H ₆ N ₂ O ₃ , ZVM1VQ
hydantoin, 252	C ₃ H ₄ N ₂ O ₂ , T5MVMV EHV
hydrazodicarbamide, 247	C ₂ H ₆ N ₄ O ₂ , ZVM1VQ
5,5'-hydrazotetrazole, 251	C ₂ H ₄ N ₁₀ , T5MNNNJ EMM- ET5MNNNJ
hydroquinone, 230	C ₆ H ₆ O ₂ , QR DQ
hydrosorbic acid, 235	C ₆ H ₁₀ O ₂ , QV2U3
DL-β-hydroxybutyric acid, 235	C ₄ H ₈ O ₃ , QY1VQ
3(a)-hydroxy-trans-decalin-2(a) acetic acid lactone (boat), 242	C ₁₂ H ₁₈ O ₂ , T C566 DOVTJ A&CCI B&A
3(e)-hydroxy-trans-decalin-2(e) acetic acid lactone (chair), 242	C ₁₂ H ₁₈ O ₂ , T C566 DOVTJ -A&I -B&ACC
hydroxyisobutyric acid, 235	C ₄ H ₈ O ₃ , QXVQ
5-hydroxy-1-pentanol, 232	C ₅ H ₁₀ O ₂ , VH4Q
L-hydroxyproline, 248	C ₅ H ₈ NO ₃ , T5MTJ BVQ DQ -A&B -B&D
8-hydroxyquinoline, 254	C ₉ H ₇ NO, T66 BNJ JQ
5-hydroxytetrazole, 251	CH ₂ N ₄ O, T5MNNNJ EQ
hydurilic acid, 254	C ₈ H ₆ N ₄ O ₆ , T6VMVMV FHJ F- 2
hypoxanthine, 252	C ₅ H ₄ N ₄ O, T56 BM DN FVM INJ
I	
imidazole, 252	C ₃ H ₄ N ₂ , T5M CNJ
indigotin, 254	C ₁₆ H ₁₀ N ₂ O ₂ , T56 BMYVJ C- 2U

Compound name, page	Empirical formula, WLN
indole, 254	C ₈ H ₇ N, T56 BMJ
inulin, 277	
inulin hexaacetate, 277	
insulin, 277	
isatide, 254	C ₁₆ H ₁₂ N ₂ O ₄ , T56 BMV DHJ DQ D- 2
isatin, 254	C ₈ H ₅ NO ₂ , T56 BMVVJ
isobutyl alcohol, see 2-methyl-1-propanol	
isobutylamine, 245	C ₄ H ₁₁ N, Z1Y
DL-isoleucine, 248	C ₆ H ₁₃ NO ₂ , QVYZY2
L-isoleucine, 248	C ₆ H ₁₃ NO ₂ , QVYZY2 -BA
isopropyl alcohol, see 2-propanol	
isopropylamine, 245	C ₃ H ₉ N, ZY
isoquinoline, 254	C ₉ H ₇ N, T66 CNJ
L-isoserine, 248	C ₃ H ₇ NO ₃ , Z1YQVQ -A
isouric acid, 252	C ₅ H ₄ N ₄ O ₆ , T6VMVMV FHJ FMCN
iso-uroporphyrin (II) octamethyl ester, 256	C ₄₈ H ₃₆ N ₄ O ₁₆ , T D5 15 N5-16-5 A D- I- N- AM D-N I-M N-NJ EIYVO1&VO1 F JIYVO1&VO1 K OIYVO1& VO1 P TIYVO1&VO1 U C ₅ H ₆ O ₄ , QVYU1&IVQ
itaconic acid, 237	
α-ketoglutaric acid, 236	
γ-ketovaleric acid, see levulinic acid	
	K
	C ₅ H ₆ O ₅ , QVV2VQ
	L
D-lactic acid, 235	C ₃ H ₆ O ₃ , QYVQ -A
DL-lactic acid, 235	C ₃ H ₆ O ₃ , QYVQ
actide, 241	C ₆ H ₈ O ₄ , T6OV DOVTJ C F
β-lactose, 243	C ₁₂ H ₂₂ O ₁₁ , T6OTJ BQ CQ DQ F1Q EO- BT6OTJ CQ DQ EQ F1Q -A&CE -B&BDF -A&C -B&BDEF
α-lactose monohydrate, 243	C ₁₂ H ₂₄ O ₁₂ , T6OTJ BQ CQ DQ F1Q EO- BT6OTJ CQ DQ EQ F1Q -A&BCE -B&BDF -A&C -B&BDEF &QH
lactose octaacetate, 243	C ₂₈ H ₃₈ O ₁₉ , T6OTJ BOV1 COV1 DOV1 FIOV1 EO- BT6OTJ COV1 DOV1 EVO1 FIOV1 -A&CE -B&BDF -A&C -B&BDEF
lauric acid, 234	C ₁₂ H ₂₄ O ₂ , QV11
D-leucine, 248	C ₆ H ₁₃ NO ₂ , QVYZIY -A
DL-leucine, 248	C ₆ H ₁₃ NO ₂ , QVYZIY
L-leucine, 248	C ₆ H ₁₃ NO ₂ , QVYZIY -R
leucine anhydride, 250	C ₁₂ H ₂₂ N ₂ O ₂ , T6MV DMVTJ CIY FIY
L-(+)-leucine methyl ester salt of (+)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3'), 249	C ₃₆ H ₄₄ N ₂ O ₁₀ , L66J CQ DVQ B- 2 -D &1Y&1YZVO1 -A 2
L-(+)-leucine methyl ester salt of (-)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3'), 249	C ₃₆ H ₄₄ N ₂ O ₁₀ , L66J CQ DVQ B- 2 -L &1Y&1YZV01 -A 2
DL-leucylglycine, 250	C ₈ H ₁₆ N ₂ O ₃ , QV1MVYZIY
leucylglycylglycine, 250	C ₁₀ H ₁₈ N ₃ O ₄ , QV1MV1MVYZIY
levoglucosan, 242	C ₆ H ₁₀ O ₅ , T56 A AO COTJ FQ GQ HQ -A&BG -B&EFH
levoglucosan triacetate, 242	C ₁₂ H ₁₆ O ₈ , T56 A AO COTJ FOV1 GOV1 HOV1 -A&BG -B&EFH
levulinic acid, 235	C ₅ H ₈ O ₃ , QVYV1
levulinic lactone, 241	C ₅ H ₆ O ₂ , T5OV CHJ E
linseed oil, 277	
lophine, 254	
DL-lysine, 240	C ₂₁ H ₁₆ N ₂ , T5M CNJ BR& DR& ER C ₆ H ₁₄ N ₂ O ₂ , Z4YZVQ
	M
maleic acid, 237	C ₄ H ₄ O ₄ , QV1U1VQ -C
maleic anhydride, 238	C ₄ H ₂ O ₃ , T5VOVJ
DL-malic acid, 236	C ₄ H ₆ O ₅ , QVYQ1VQ
L-malic acid, 236	C ₄ H ₆ O ₅ , QVYQ1VQ -B
malonamide, 246	C ₃ H ₆ N ₂ O ₂ , ZV1VZ
malonic acid, 236	C ₃ H ₄ O ₄ , QV1VQ
maltose, 243	C ₁₂ H ₂₂ O ₁₁ , T6OTJ BQ CQ DQ F1Q EO- BT6OTJ CQ DQ EQ F1Q -A&CE -B&BDF -A&BCE -B&BDF
β-maltose monohydrate, 243	C ₁₂ H ₂₄ O ₁₂ , T6OTJ BQ CQ DQ F1Q EO- BT6OTJ CQ DQ EQ F1Q -A&CE -B&BDF -A&BCE -B&BDF &QH
maltose octaacetate, 243	C ₂₈ H ₃₈ O ₁₉ , T6OTJ BOV1 COV1 DOV1 FIOV1 EO- BT6OTJ COV1 DOV1 EVO1 FIOV1 -A&CE -B&BDF -A&BCE -B&BDF
DL-mandelic acid, 238	C ₈ H ₈ O ₃ , QYR&VQ
L-mandelic acid, 238	C ₈ H ₈ O ₃ , QYR&VQ -B
D-mannitol, 231	C ₆ H ₁₄ O ₆ , Q1YQYQ 2 -BBAA
mannitol triacetate, 244	C ₁₂ H ₂₀ O ₆ , T5O COTJ B D- 2 D ET5O COTJ B
mannitol triformate, 244	C ₉ H ₁₄ O ₆ , T5O COTJ D- 2 D ET5O COTJ
D-mannonic acid-1,4,3,6-dilactone, 241	C ₆ H ₆ O ₆ , T55 BOV FOTVJ DQ HQ -B&ADEH
D-mannonic acid-γ-lactone, 241	C ₆ H ₁₀ O ₆ , T5OVTJ CQ DQ EYQ1Q -A&E -B&CD -A
D-mannose, 242	C ₆ H ₁₂ O ₆ , T6OTJ BQ CQ DQ EQ F1Q -A&E -B&CDF
melamine, 252	C ₃ H ₆ N ₆ , T6N CN ENJ BZ DZ FZ
melezitose, 244	C ₁₈ H ₃₂ O ₁₆ , T6OTJ B1Q CQ DQ EQ FO- 2 B CT5OTJ B1Q DQ E1Q -A&BD -B&CEF -A&D -B&BCE -A&BD -B&CEF
mesaconic acid, 237	C ₅ H ₆ O ₄ , QVYU1VQ -T

Compound name, page	Empirical formula, WLN
meso-1,2,3,4-butanetetrol, 231	C ₄ H ₁₀ O ₄ , Q1YQYQ1Q -AA
meso-erythritol, see meso-1,2,3,4-butanetetrol	
mesoporphyrin (IX) dimethyl ester, 256	C ₃₆ H ₃₂ N ₄ O ₄ , T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-NJ E2VO1 F J2 K O2 P T U2VO1
meso-tartramide, 246	C ₄ H ₈ N ₂ O ₄ , ZVYQYQVZ -AA
meso-tartaric acid, 236	C ₄ H ₆ O ₆ , QVYQYQVQ -AA
mesoxalic acid, 235	C ₃ H ₄ O ₆ , QVXQQVQ
methanal, see formaldehyde	
methane, 226	CH ₄ 1H
methanethiol, 256	CH ₄ S, SH1
methanoic acid, see formic acid	
methanol, 229	CH ₄ O, Q1
L-methionine, 248	C ₅ H ₁₁ NO ₂ S, QVYZ2S1 -B
5-methoxytetrazole, 251	C ₂ H ₄ N ₄ O, T5MNNNJ EO1
methyl acetate, 238	C ₃ H ₆ O ₂ , 1VO1
methyl alcohol, see methanol	
methyl allantoin, 253	C ₅ H ₈ N ₄ O ₃ , T5MVMV EHJ EMVZ E
methylamine, 245	CH ₅ N, Z1
methylamine nitrate, 245	CH ₆ N ₂ O ₃ , Z1 & H-N-O3
1-methyl-5-aminotetrazole, 251	C ₂ H ₅ N ₅ , T5NNNNJ A EZ
2-methyl-5-aminotetrazole, 251	C ₂ H ₅ N ₅ , T5NNNNJ B EZ
5-methylaminotetrazole, 251	C ₂ H ₅ N ₅ , T5MNNNJ EM1
N-methylamine, 246	C ₇ H ₉ N, 1MR
methyl benzoate, 239	C ₈ H ₈ O ₂ , 1OVR
methyl caprate, 238	C ₁₁ H ₂₂ O ₂ , 9VO1
methyl caproate, 238	C ₇ H ₁₄ O ₂ , 5VO1
5-methylcaprolactam, 254	C ₇ H ₁₃ NO, T7MVTJ E
7-methylcaprolactam, 254	C ₇ H ₁₃ NO, T7MVTJ G
N-methylcaprolactam, 254	C ₇ H ₁₃ NO, T7NVTJ A
methyl caprylate, 238	C ₉ H ₁₈ O ₂ , 7VO1
methyl elaidate, 238	C ₁₉ H ₃₆ O ₂ , 9U8VO1 -T
methyl enanthate, 238	C ₈ H ₁₆ O ₂ , 6VO1
β-methylene-β-propiolactone, 241	C ₄ H ₄ O ₂ , T4VOY DHJ CUI
methyl ethyl ether, 231	C ₃ H ₈ O, 2O1
methyl ethyl heptanone lactone (racemic), 242	C ₁₀ H ₁₆ O ₃ , T5OVTJ D2V1 E E
5-methyl-5-ethyl hydantoin, 253	C ₆ H ₁₀ N ₂ O ₂ , T5MVMV EHJ E2 E
methyl ethyl ketone, see butanone	
methyl formate, 238	C ₂ H ₄ O ₂ , VHO1
β-methyl-D-glucofuranoside, 249	C ₇ H ₁₄ O ₆ , T5OTJ BYQ1Q CQ DQ EO1 -A&BCE -B&D -B
α-methyl-D-glucopyranoside, 242	C ₇ H ₁₄ O ₆ , T6OTJ BO1 CQ DQ EQ F1Q -A&BCE -B&DF
β-methyl-D-glucopyranoside, 242	C ₇ H ₁₄ O ₆ , T6OTJ BO1 CQ DQ EQ F1Q -A&CE -B&BDF
5-methylhydantoin, 252	C ₄ H ₈ N ₂ O ₂ , T5MVMV EHJ E
4-methylhydrouracil, 253	C ₅ H ₆ N ₂ O ₂ , T6MVMVTJ F
7-methylhypoxanthine, 253	C ₆ H ₆ N ₄ O, T56 BN DN FN HMVJ B
α-methylindole, 254	C ₉ H ₉ N, T56 BMJ C
β-methyl indole, see skatole	
methyl laurate, 238	C ₁₃ H ₂₆ O ₂ , 11VO1
methyl myristate, 238	C ₁₅ H ₃₀ O ₂ , 13VO1
methyl oleate, 238	C ₁₉ H ₃₆ O ₂ , 9U8VO1 -C
methyl pelargonate, 238	C ₁₀ H ₂₀ O ₂ , 8VO1
methyl pentadecylate, 238	C ₁₆ H ₃₂ O ₂ , 14VO1
2-methyl phenol, see o-cresol	
3-methyl phenol, see m-cresol	
4-methyl phenol, see p-cresol	
1-methyl-5-phenyltetrazole, 254	C ₈ H ₈ N ₄ , T5NNNNJ A ER
methyl pheophorbide a, 256	C ₃₀ H ₃₆ N ₄ O ₃ , T-T55 BNY FV HY CHJ D CVO1 HU- AT5YMYTJ D E2VO1 CU1- ET5NYJ CIU1 D BUI- BT5MJ C D2 E1U- C-16-J
	C ₃₆ H ₃₆ N ₄ O ₆ , T-T55 BNY FV HY CHJ D GVO1 HU- AT5YMYTJ D E2VO1 CU1- ET5NYJ CIU1 D BUI- BT5MJ CVH D2 E1U- C-16-J
	C ₆ H ₁₁ NO, T6NVTJ A
	C ₄ H ₁₂ N ₂ , ZX1Z
	C ₄ H ₁₀ O, Q1Y
	C ₄ H ₁₀ O, QX
	C ₆ H ₆ N ₄ , T56 BN DN FN HNJ B
	C ₆ H ₇ N, T6NJ B
	C ₆ H ₇ N, T6NJ C
	C ₆ H ₇ N, T6NJ D
	C ₅ H ₉ NO, T5NVTJ A
	C ₈ H ₈ O ₃ , QR BVO1
	C ₄ H ₅ NS, T5N CSJ E
	C ₅ H ₆ S, T5SJ B
	C ₅ H ₆ S, T5SJ C
	C ₁₄ H ₂₈ O ₂ , 12VO1
	C ₁₂ H ₂₄ O ₂ , 10VO1
	C ₅ H ₆ N ₂ O ₂ , T6MVMVJ F
	C ₆ H ₁₂ O ₂ , 4VO1
	C ₁₇ H ₂₁ NO ₄ , T B6566 B6/CO 4ABBC R BX HO PN DU GHT&TTJ FQ JQ P -A&FO -B&BCG &QH
methyl pheophorbide b, 256	
N-methyl piperidone, 253	
2-methyl-1,2-propanediamine, 245	
2-methyl-1-propanol, 229	
2-methyl-2-propanol, 229	
methyl n-propyl ketone, see 2-pentanone	
7-methyl purine, 253	
2-methylpyridine, 253	
3-methylpyridine, 253	
4-methylpyridine, 253	
N-methylpyrrolidone, 253	
α-methyl quinoline, see quinaldine	
methyl salicylate, 239	
methyl theobromine, see caffeine	
4-methylthiazole, 257	
2-methylthiophene, 257	
3-methylthiophene, 257	
methyl tridecylate, 238	
methyl undecylate, 238	
4-methyluracil, 253	
5-methyluracil, see thymine	
methyl valerate, 238	
milk casein, 277	
morphine monohydrate, 251	

Compound name, page	Empirical formula, WLN
mucic acid, 236	C ₆ H ₁₀ O ₈ , QVYQYQ 2 -ABBA
murexide, 254	C ₈ H ₈ N ₆ O ₆ , T6MVMVYVJ EUN- ET6MVMVJ FQ &ZH
myristic acid, 234	C ₁₄ H ₂₈ O ₂ , QV13
N	
naphthacene, 228	C ₁₈ H ₁₂ , L E6 C666J
naphthalene, 227	C ₁₀ H ₈ , L66J
narceine dihydrate, 251	C ₂₃ H ₃₁ NO ₁₀ , T56 BO DO CHJ FO1 G1VR BVQ CO1 DO1& H2N1&1 &QH &QH
narcotine, 251	C ₂₂ H ₂₈ NO ₇ , T C566 DO FO KN EH&&TJ JO1 K J- DT56 BVO DHJ HO1 IO1
nicotine, 254	C ₁₀ H ₁₄ N ₂ , T6NJ C- BT5NTJ A
nitrotriacetic acid, 248	C ₆ H ₉ NO ₆ , QV1 3N
nitroaminoguanidine, 247	CH ₅ N ₅ O ₂ , ZMYUM&MNW
nonanoic acid, see pelargonic acid	
norleucine, see α-aminocaproic acid	
O	
octadecanoic acid, see stearic acid	
octaethyl porphyrin, 256	C ₃₆ H ₄₈ N ₄ , T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-NJ E2 F2 J2 K2 O2 P2 T2 U2
<i>n</i> -octaldehyde, 232	C ₈ H ₁₆ O, VH7
1-octanal, see <i>n</i> -octaldehyde	
octanoic acid, see caprylic acid	
oleic acid, 235	
olive oil, 277	
DL-ornithine, 248	C ₁₈ H ₃₄ O ₂ , QV8U9 -C
oxacyclobutane, 244	C ₅ H ₁₂ N ₂ O ₂ , Z3YZVQ
oxalic acid, 236	C ₂ H ₂ O ₄ , T4OTJ
oxalic acid dihydrate, 236	C ₂ H ₂ O ₄ , QVVQ
oxamic acid, 246	C ₂ H ₂ NO ₃ , ZVVQ
oxamide, 246	C ₂ H ₄ N ₂ O ₂ , ZVVZ
oxindole, 254	C ₈ H ₇ NO, T56 BMV DHJ
6-oxypurine, see hypoxanthine	
8-oxypurine, 252	C ₅ H ₄ N ₄ O, T56 BMVM FN HNJ
P	
palmitic acid, 234	C ₁₆ H ₃₂ O ₂ , QV15
papaverine, 251	C ₂₀ H ₂₁ NO ₄ , T66 CNJ B1R CO1 DO1& HO1 IO1
parabanic acid, 252	C ₃ H ₂ N ₂ O ₃ , T5MVMVJ
paraglobulin, 277	
paraldehyde, 232	C ₆ H ₁₂ O ₃ , T6O CO EOTJ B D F
pelargonic acid, 233	C ₉ H ₁₈ O ₂ , QV8
pentaerythritol, 231	C ₅ H ₁₂ O ₄ , Q1 4X
1-pentanal, see <i>n</i> -valeraldehyde	
<i>n</i> -pentane, 226	C ₅ H ₁₂ , 5H
1-pentanethiol, 257	C ₅ H ₁₂ S, SH5
pentanoic acid, see valeric acid	
1-pentanol, 229	C ₅ H ₁₂ O, Q5
2-pentanone, 233	C ₅ H ₁₀ O, 3V1
3-pentanone, 233	C ₅ H ₁₀ O, 2V2
D-perseitol, 231	C ₇ H ₁₆ O ₇ , Q1/YO/ 51Q -ABBAA
perylene, 228	C ₂₀ H ₁₂ , L666 L6 K6 2AL TJ
phenacetin, 247	C ₁₀ H ₁₃ NO ₂ , 2OR DMV1
phenaceturic acid, 249	C ₁₀ H ₁₁ NO ₃ , QV1MV1R
phenanthrene, 227	C ₁₄ H ₁₀ , L B666J
phenazine, 254	C ₁₂ H ₈ N ₂ , T C666 BN INJ
phenol, 230	C ₆ H ₆ O, QR
phenoxyacetic acid, 238	C ₈ H ₈ O ₃ , QV1OR
phenylacetic acid, 238	C ₈ H ₈ O ₂ , QV1R
DL-phenylalanine, 249	C ₉ H ₁₁ NO ₂ , QVYZ1R
L-phenylalanine, 249	C ₉ H ₁₁ NO ₂ , QVYZ1R -B
phenylalanine anhydride, 250	C ₁₈ H ₁₈ N ₂ O ₂ , T6MV DMVTJ C1R& FIR
phenylalanine- <i>N</i> -carboxylic acid anhydride, 250	C ₁₀ H ₈ NO ₃ , T5MVOV EHJ E1R
DL-phenylalanine- <i>N</i> -carboxylic acid dimethyl ester, 249	C ₁₂ H ₁₅ NO ₄ , 1OVY1R&MVO1
phenylalanine polypeptide, 277	
1-phenyl-5-aminotetrazole, 253	C ₇ H ₇ H ₅ , T5NNNNJ AR& EZ
5-phenylaminotetrazole, 253	C ₇ H ₇ N ₅ , T5MNNNJ EMR
DL-phenylglyceric acid, 238	C ₉ H ₁₀ O ₄ , QYR&YQVQ
α-phenyl glycine, 249	C ₈ H ₉ NO ₂ , ZYR&VQ
<i>N</i> -phenyl glycine, 249	C ₈ H ₉ NO ₂ , QV1MR
phenylglyoxylic acid, 237	C ₈ H ₆ O ₃ , QVVR
1-phenyl-5-hydroxytetrazole, 253	C ₇ H ₆ N ₄ O, T5NNNNJ AR& EQ
phenyl methyl sulfide, 257	C ₇ H ₈ S, 1SR
1-phenyl-5-methyltetrazole, 254	C ₈ H ₈ N ₄ , T5NNNNJ AR& E
2-phenyl-5-methyltetrazole, 254	C ₈ H ₈ N ₄ , T5NNNNJ BR& E
α-phenylpyrrole, 254	C ₁₀ H ₉ N, T5MJ BR
<i>N</i> -phenylpyrrole, 254	C ₁₀ H ₉ N, T5NJ AR
1-phenyltetrazole, 253	C ₇ H ₆ N ₄ , T5NNNNJ AR
5-phenyltetrazole, 253	C ₇ H ₆ N ₄ , T5MNNNJ ER
4-phenyl uracil, 254	C ₁₀ H ₈ N ₂ O ₂ , T6MVMVJ FR

Compound name, page	Empirical formula, WLN
pheoporphyrin <i>a</i> ₅ dimethyl ester, 256	C ₃₆ H ₃₈ N ₄ O ₅ , T-T55 BNY FV HY GHJ D GVO1 HU- AT5YMYJ D E2VO1 CU1- ET5NYJ C2 D BU1- BT5MJ C D2 EU- C-16-J
pheopurpurin 18 monomethyl ester, 256	C ₃₄ H ₃₆ N ₄ O ₅ , T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-N&&&&TJ CVO1 EVQ F J2 K O1U1 P T U2VQ
phthalamide, 246	C ₈ H ₈ N ₂ O ₂ , ZVR BVZ
<i>m</i> -phthalic acid, 237	C ₈ H ₆ O ₄ , QVR CVQ
<i>o</i> -phthalic acid, 238	C ₈ H ₆ O ₄ , QVR BVQ
<i>p</i> -phthalic acid, 238	C ₈ H ₆ O ₄ , QVR DVQ
phylloerthyrin monomethyl ester, 255	C ₃₄ H ₃₆ N ₄ O ₅ , T-T55 BNY FV HY GHJ D HU- AT5YMYJ D E2VO1 CU1- ET5NYJ C2 D BU1- BT5MJ C D2 EU- C-16-J
γ-phylloporphyrin monomethyl ester, 255	C ₃₃ H ₃₈ N ₄ O ₂ , T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-NJ C F J2 K O2 P T U2VO1
phyllopyrrole, 254	C ₉ H ₁₅ N, T5MJ B C2 D E
picolinic acid, 253	C ₆ H ₅ NO ₂ , T6NJ BVQ
piperazine, 252	C ₄ H ₁₀ N ₂ , T6M DMTJ
piperazine hexahydrate, 252	C ₄ H ₂₂ N ₂ O ₆ , T6M DMTJ &/QH 6
piperidine, 253	C ₅ H ₁₁ N, T6MTJ
α-piperidone, 253	C ₅ H ₉ NO, T6MVTJ
poppy seed oil, 277	
potato starch, 277	
Δ ₄ -pregnene-3,20-dione, 241	C ₂₁ H ₃₀ O ₂ , L E5 B666 OV MUTJ A E FV1 -A&BI -B&AEFJ
Δ ₄ -pregnene-3,20-dione-21-ol, 241	C ₂₁ H ₃₀ O ₃ , L E5 B666 OV MUTJ A E FV1Q -A&BI -B&AEFJ
Δ ₄ -pregnene-3,20-dione-11β,17α,21-triol, 241	C ₂₁ H ₃₀ O ₅ , L E5 B666 OV MUTJ A CQ E FV1Q FO -A&BI -B&ACEFJ
Δ ₄ -pregnene-3,11,20-trione,17α,21-diol, 240	C ₂₁ H ₂₈ O ₅ , L E5 B666 CV OV MUTJ A E FV1Q FQ -A&BI -B&AEFJ
progesterone, see Δ ₄ -pregnene-3,20-dione	
DL-proline, 248	C ₅ H ₉ NO ₂ , T5MTJ BVQ
1-propanal, see <i>n</i> -propionaldehyde	
propane, 226	C ₃ H ₈ , 3H
1,2-propanediamine, 245	C ₃ H ₁₀ N ₂ , ZY1Z
1,2-propanediol, 231	C ₃ H ₈ O ₂ , QY1Q
1,3-propanediol, 231	C ₃ H ₈ O ₂ , Q3Q
1,3-propanedithiol, 256	C ₃ H ₆ S ₂ , SH3SH
1-propanethiol, 256	C ₃ H ₈ S, SH3
1,2,3-propanetriol, 231	C ₃ H ₈ O ₃ , Q1YQ1Q
propanoic acid, see propionic acid	
1-propanol, 229	C ₃ H ₈ O, Q3
2-propanol, 229	C ₃ H ₈ O, QY
propanone, 232	C ₃ H ₆ O, IV1
β-propiolactone, 241	C ₃ H ₄ O ₂ , T4OVTJ
<i>n</i> -propionaldehyde, 232	C ₃ H ₆ O, VH2
propionamide, 246	C ₃ H ₇ NO, ZV2
propionic acid, 233	C ₃ H ₆ O ₂ , QV2
<i>n</i> -propyl alcohol, see 1-propanol	
<i>n</i> -propyl amine, 245	C ₃ H ₉ N, Z3
propylene glycol, see 1,2- and 1,3-propanediol	
protoporphyrin, 255	C ₃₄ H ₃₄ N ₄ O ₄ , T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-NJ E2VQ F J1U1 K O1U1 P T U2VQ
protoporphyrin dimethyl ester, 256	C ₃₆ H ₃₈ N ₄ O ₄ , T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-NJ E2VO1 F J1U1 K O1U1 P T U2VO1
pseudouric acid, 253	C ₅ H ₆ N ₂ O ₄ , T6VMVMV FHJ FMVZ
pyrazine, 252	C ₄ H ₄ N ₂ , T6N DNJ
pyrazole, 252	C ₃ H ₄ N ₂ , T5MNJ
pyrene, 228	C ₁₆ H ₁₀ , L666 B6 2AB PJ
pyridazine, 252	C ₄ H ₄ N ₂ , T6NNJ
pyridine, 252, 253	C ₅ H ₅ N, T6NJ
pyrimidine, 252	C ₄ H ₄ N ₂ , T6N CNJ
pyrocatechol, 230	C ₆ H ₆ O ₂ , QR BQ
pyromucic acid, see 2-furoic acid	
pyropheophorbide <i>a</i> monomethyl ester, 255	C ₃₄ H ₃₆ N ₄ O ₃ , T-T55 BNY FV HY GHJ D HU- AT5YMYJ D E2VO1 CU1- ET5NYJ C2 D BU1- BT5MJ C D2 EU- C-16-J
pyrrolaldehyde, 253	C ₅ H ₈ NO, T5MJ BVH
pyrrolaldoxime, 253	C ₅ H ₈ N ₂ O, T5MJ BIUNQ
pyrrole, 252	C ₄ H ₅ N, T5MJ
pyrrolidine, 252	C ₄ H ₉ N, T5MTJ
α-pyrrolidone, 252	C ₄ H ₇ NO, T5MVTJ
pyrroporphyrin (XV) monomethyl ester, 255	C ₃₂ H ₃₆ N ₄ O ₂ , T D5 I5 N5-16-5 A D- I- N- AM D-N I-M N-NJ E2 F J K2VO1 P T2 U
pyruvic acid, 235	C ₃ H ₄ O ₃ , QVV1
pyruvile, see methyl allantoin	
quinaldine, 254	
quinidine, 251	
quinine, 251	
quinoline, 254	
	Q
	C ₁₀ H ₉ N, T66 BNJ C
	C ₂₀ H ₂₄ N ₂ O ₂ , T66 BNJ HO1 EYQ- DT66 A B CNTJ AIU1 -A -A&DF -B&A
	C ₂₀ H ₂₄ N ₂ O ₂ , T66 BNJ HO1 EYQ- DT66 A B CNTJ AIU1 -B -A&F -B&AD
	C ₈ H ₇ N, T66 BNJ

Compound name, page	R	Empirical formula, WLN
raffinose, 244		C ₁₈ H ₃₂ O ₁₆ , T60TJ B1Q CQ DQ EQ FO1- BT60TJ CQ DQ EQ FO- BT50TJ B1Q CQ DQ EQ EQ1 -A&BCD -B&EF -A&BD -B&CEF -A&D -B&BCE
raffinose pentahydrate, 244		C ₁₈ H ₄₂ O ₂₁ , T60TJ B1Q CQ DQ EQ FO1- BT60TJ CQ DQ EQ FO- BT50TJ B1Q CQ DQ EQ EQ1 -A&BCD -B&EF -A&BD -B&CEF -A&D -B&BCE &/QH 5
resorcinol, 230		C ₆ H ₆ O ₂ , QR CQ
β-L-rhamnose, 242		C ₆ H ₁₂ O ₅ , T60TJ BQ CQ DQ EQ F -A&BCDF -B&E
α-L-rhamnose monohydrate, 242		C ₆ H ₁₄ O ₆ , T60TJ BQ CQ DQ EQ F -A&CDF -B&BE &QH
rhamnose triacetate, 242		C ₁₄ H ₂₀ O ₉ , T60TJ BQ COV1 DOV1 EOVI F A&CDF -B&E
rhodoporphyrin (XV) dimethyl ester, 256		C ₃₄ H ₃₈ N ₄ O 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 ₄ O 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		C ₅ H ₁₀ O ₅ , T60TJ BQ CQ DQ EQ -A&CDE -B&B
rice starch, 277		
rye bread, 277		
saccharinic acid lactone, 241		
salicylaldehyde, 232		
salicylic acid, 237		
sarcosine, 247		
sarcosine-N-carboxylic acid anhydride, 250		
sarcosine polypeptide, 277		
seed extracts, 277		
L-serine, 248		
serine anhydride, 250		
serylserine, 250		
skatole, 254		
sorbic acid, 235		
L-sorbose, 242		
stachyose, 244		
stearic acid, 234		
starch, 277		
starch hexaacetate, 277		
strychnine, 251		
succinamide, 246		
succinic acid, 236		
succinic anhydride, 238		
sucrose, 243		
sucrose octaacetate, 243		
DL-tartaric acid, 236		
DL-tartaric acid monohydrate, 236		
L-tartaric acid, 236		
L-tartramide, 246		
taurine, see 2-aminoethane-1-sulfonic acid		
terebic acid, 241		
testosterone, see Δ ₄ -androsterone-3-one-17β-ol		
tetracene, see naphthacene		
tetraconic acid, 237		
tetradecanoic acid, see myristic acid		
tetrahydrofuran, 244		
tetrahydrofurfuryl alcohol, 244		
tetrahydropyran, 244		
1,2,5,6-tetrahydropyridine, 253		
tetramethylene-1,4-diamine-sebacic acid adduct, 248		
tetramethylthiuram disulfide, 257		
tetramethylthiuram monosulfide, 257		
α-tetramylose, 244		
tetrazole, 251		
1-(5-tetrazolyl)-4-guanyl-tetrazene monohydrate, 252		
5-tetrazolylurethan, 252		
thebaine, 251		
theobromine, 253		
thiacyclobutane, 256		
thiacyclohexane, 257		
	S	
		C ₆ H ₁₀ O ₅ , T50VTJ CQ C DQ EQ1
		C ₇ H ₆ O ₂ , VHR BQ
		C ₇ H ₆ O ₃ , QVR BQ
		C ₃ H ₇ NO ₂ , QV1MI
		C ₄ H ₅ NO ₃ , T5NVOV EHJ A
		C ₃ H ₇ NO ₃ , QVYZ1Q -B
		C ₆ H ₁₀ N ₂ O ₄ , T6MV DM EVTJ C1Q F1Q
		C ₆ H ₁₂ N ₂ O ₅ , QVY1QM VYZ1Q
		C ₉ H ₉ N, T56 BMJ D
		C ₆ H ₈ O ₂ , QV1U2U2
		C ₆ H ₁₂ O ₆ , Q1YQYQYQV1Q -ABA
		C ₂₄ H ₄₂ O ₂₁ , T60TJ B1Q CQ DQ EQ/ FO1- BT60TJ CQ DQ EQ/ 2 FO- BT50TJ B1Q CQ DQ EQ1/ -A&BCD -B&EF/ 2 -A&BD -B&CEF -A&D -B&BCE
		C ₁₈ H ₃₆ O ₂ , QV17
		C ₂₁ H ₂₂ N ₂ O ₂ , T6 G56 B7 C6 E5 D 5ABCEF A& FX MNV QO VN SU AHT&&TTTTJ
		C ₄ H ₈ N ₂ O ₂ , ZV2VZ
		C ₄ H ₆ O ₄ , QV2VQ
		C ₄ H ₄ O ₃ , T5VOVTJ
		C ₁₂ H ₂₂ O ₁₁ , T60TJ B1Q CQ DQ EQ FO- BT50TJ B1Q CQ DQ EQ1 -A&BD -B&CEF -A&D -B&BCE
		C ₂₈ H ₃₈ O ₁₉ , T60TJ B1OV1 COV1 DOV1 EOVI FQ- BT50TJ B1OV1 COV1 DOV1 E1OV1 -A&BD -B&CEF -A&BD -B&CE
	T	
		C ₄ H ₆ O ₆ , QVYQYQVQ
		C ₄ H ₈ O ₇ , QVYQYQVQ &QH
		C ₄ H ₆ O ₆ , QVYQYQVQ -AB
		C ₄ H ₈ N ₂ O ₄ , ZVYQYQVZ -AB
		C ₇ H ₁₀ O ₄ , T50VTJ DVQ E E
		C ₇ H ₁₀ O ₄ , QV1YVQUY
		C ₄ H ₈ O, T50TJ
		C ₅ H ₁₀ O ₂ , T50TJ B1Q
		C ₅ H ₁₀ O, T60TJ
		C ₅ H ₉ N, T6M CUTJ
		C ₁₄ H ₃₀ N ₂ O ₄ , QV6VQ &Z4Z
		C ₆ H ₁₂ N ₂ S ₄ , 1N1&YUS&S 2
		C ₆ H ₁₂ N ₂ S ₃ , 1N1&YUS& 2S
		C ₃₈ H ₆₀ O ₃₀ , T60TJ BQ CQ DQ EQ FO1- BT60TJ CQ DQ EQ FO1- 4 BT60TJ CQ DQ EQ EQ1 / -A&BCE -B&DF/ 6
		CH ₂ N ₄ , T5MNNNJ
		C ₅ H ₈ N ₁₀ O, T5MNNNJ ENUNMMYUM &QH
		C ₄ H ₇ N ₅ O ₂ , T5MNNNJ EMVO2
		C ₁₉ H ₂₁ NO ₃ , T B6566 B6/CO 4ABBC R BX HO PN GH&&TTJ FO1 JO1 P
		C ₇ H ₈ N ₄ O ₂ , T56 BN DN FNV MVJ B F
		C ₃ H ₆ S, T4STJ
		C ₅ H ₁₀ S, T6STJ

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C₄H₈S, T5STJ
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 C₂H₆S, 1S1
 C₃H₆N₂O₂S, SUYZM1VQ
 C₃H₄N₂OS, T5MYMV EHJ BUS
 C₂H₄OS, SHV1
 C₃H₆O₂S, SHYVQ
 C₄H₄S, T5SJ
 CH₄N₂S, ZYZUS
 C₄H₈NO₃, QY&YZVQ
 C₄H₆NO₃, QY&YZVO -AA
 C₅H₆N₂O₂, T6MVMVJ E
 C₅H₈O₂ QVYU2 -T
 C₁₁H₁₃NO₃, QVYMVR B
 C₁₁H₁₃NO₃, QVYMVR D
 C₁₀H₁₁NO₃, QV1MVR C
 C₁₀H₁₁NO₃, QV1MVR B
 C₁₀H₁₁NO₃, QV1MVR D
 C₁₂H₂₂O₁₁, T6OTJ B1Q CQ DQ EQ F- 20 /-A&BD
 -B&CE/ 2
 C₁₂H₂₆O₁₃, T6OTJ B1Q CQ DQ EQ F- 20 /-A&BD
 -B&CE/ 2 &QH &QH
 C₁₂H₂₇O₄P, 4O 3PO
 C₁₂H₂₇OP, OP4&4&4
 C₁₅H₂₆O₆, L3TJ AVO 3/1Y1/
 C₁₈H₂₆O₆, L4TJ AVO 3/1Y1/
 C₆H₁₅N, 2N2&2
 C₆H₁₆N₂O₃, 2N2&2 & H-N-O3
 C₆H₁₂N₂, T66 A B CN FNTJ
 C₆H₁₅O₄P, 2O 3PO
 C₈H₁₄N₄O₅, Z1VM1VM1VM1VQ
 C₅H₈O₇, QVYQYQYQVQ
 C₁₂H₂₇O₄P, 1Y&1O 3PO
 C₃H₉N, 1N1&1
 C₃H₁₀N₂O₃, 1N1&1 & H-N-O3
 C₃H₉P, 1P1&1
 C₁₈H₁₂, L B6 H666J
 C₁₈H₁₅O₄P, RO 3PO
 C₉H₂₁N, 3N3&3
 C₉H₂₁O₄P, 3O 3PO
 C₁₁H₁₂N₂O₂, T56 BMJ DIYZVQ -B
 C₉H₁₁NO₃, QVYZ1R DQ -B

U

C₁₁H₂₀O₂, QV9U1
 C₄H₅N₃O₃, T6VMVMV FHJ FZ
 CH₄N₂O, ZVZ
 CH₅N₃O₄, ZVZ & H-N-O3

C₅H₄N₄O₃, T56 BMVM FMVMVJ

V

C₅H₁₀O, VH4
 C₅H₁₀O₂, QV4
 C₅H₁₁NO₃, QVYZY
 C₅H₁₁NO₃, QVYZY -B
 C₈H₁₄N₂O₂, T6MV DMVTJ CY F
 C₁₁H₂₀N₂O₂, T6MV DMVTJ CY F1Y
 C₁₄H₂₀N₂O₃, QVY1R&MVYZY
 C₁₄H₁₈N₂O₂, T6MV DMVTJ CY F1R
 C₃₄H₃₆N₄O₄, T D5 I5 N5-16-5 A D- I- N- AM D-N I-M
 N-NJ EVO1 F J2 K O1U1 P T U2VO1

C₇H₇N, T6NJ B1U1

W

X

C₅H₄N₄O₂, T56 BM DN FMVMVJ
 C₅H₁₂O₅, Q1YQYQYQ1Q -ABA
 C₅H₁₀O₅, T6OTJ BQ CQ DQ EQ -A&BCE -B&D

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