Revised Group Additivity Values for Enthalpies of Formation (at 298 K) of Carbon–Hydrogen and Carbon–Hydrogen–Oxygen Compounds

N. Cohen

Thermochemical Kinetics Research, 6507 SE 31st Avenue, Portland, Oregon 97202-8627

Received January 17, 1996; revised manuscript received September 4, 1996

A program has been undertaken for the evaluation and revision of group additivity values (GAVs) necessary for predicting, by means of Benson's group additivity method, thermochemical properties of organic molecules. This review reports on the portion of that program dealing with GAVs for enthalpies of formation at 298.15 K (hereinafter abbreviated as 298 K) for carbon–hydrogen and carbon–hydrogen–oxygen compounds. A complete database of experimental data for gas, liquid, and crystal (solid) phase enthalpies of formation is presented. The GAVs, ring strain corrections, and non-nearest neighbor interactions derived from the database are presented in tabular form, together with a description of their evaluation and comments on reliability, uncertainties, and missing or questionable data.

Key words: enthalpy of formation; estimation; group additivity; organic compounds; thermochemical properties.

Contents

List of Tables

1. Introduction

The importance of reliable and conveniently accessible thermochemical data (enthalpies of formation, entropies, and heat capacities) is universally accepted among both scientists and engineers. It is also accepted that the range of molecules of possible interest will, for the foreseeable future, exceed by orders of magnitude the number of compounds that can be measured in the laboratory. Hence, simple but reliable techniques are desirable for estimating thermochemical properties of species for which experimental data are not available. A number of methods have been developed in recent years; while there is not unanimous agreement regarding the best method, it seems generally agreed that one of the best (if not *the* best) is that of group additivities, especially as developed by Benson and co-workers.[1] Not only is the method fairly easy to apply, but it usually can estimate properties with an uncertainty no larger than typical experimental uncertainties. In addition to containing a description of the method, Ref. 1 tabulates the best available group additivity values (GAVs) for gas phase properties as of 1976.

Under a contract from the National Institute of Standards and Technology (NIST), we have undertaken a program for the evaluation and revision of GAVs necessary for predicting, by means of Benson's method, thermochemical properties of organic molecules.

2. Results and Procedure

2.1. Enthalpies of Formation

Numerous tabulations of thermochemical properties (including enthalpies of formation, $\Delta_f H$) of organic compounds have been published. The starting point for most subsequent tabulations has been "Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds," by Rossini *et al.*[2] However, this compilation combined experimental values with calculated and extrapolated ones in a manner that did not always make clear which were which. Stull, Westrum, and Sinke (SWS)[3] perpetuated this uncertainty in their tabulations of thermochemical properties

in the now-familiar JANAF-like format. These important references have been cited as primary sources in more recent compilations, so that now one is often hard-pressed to determine to what extent a particular compilation is dependent on nonexperimental values. This issue gains in importance when one tries to develop empirical methods for predicting thermochemical properties, as in the group additivity method; if all the Rossini and SWS values are thrown into the hopper, one in effect is fitting to already fitted values. Cox and Pilcher[4] began a program to establish the experimental database anew, and to clarify the question of what exactly has been measured and what has not. That study culminated in the monograph by Pedley *et al.*, *Thermochemical Data of Organic Compounds*[5] (PNK). That compilation is still the soundest starting point for any compilation of experimental enthalpy of formation data.[6]

Several workers have turned to Benson's group additivity method for predicting thermochemical properties. An exemplary model is Stein's computer program, available through NIST.[7] However, such programs and projects often build on previous evaluations in a way that does not always ensure mutual consistency of all of the separate parts of the evaluation. For example, most group values are derived in stepwise fashion, starting with groups of the alkanes. If the alkane group values are updated, almost all other group values will be affected. There is thus a clear need to reestablish a uniformly derived set of GAV evaluations. Hence, the motivation for the present project.

Our approach was similar to that of others in that we began by deriving GAVs for the alkane groups using as a database all the alkanes themselves.[8] The alkane groups, together with the derived values for all three phases, are shown in the first section of Table 1. With these values fixed, we then turned to all alkenes to derive GAVs necessary for those compounds. These groups and their derived GAVs are listed in the second section of Table 1. These were followed in steps by alkynes and then aromatics and polycyclics together. Gas, liquid, and crystal phase GAVs were derived in separate but parallel exercises. After all the carbon–hydrogen groups were evaluated, carbon–hydrogen–oxygen groups were addressed.

The GAVs developed in this report are based solely on experimental data, not on calculated values. While there are many computational schemes (including group additivity) that are relatively successful in predicting enthalpies of formation, it did not seem appropriate to use them to derive GAVs. Our enthalpy database, therefore, omits some species included in other compilations (e.g., SWS) because of that rigorous constraint. The reliability of the GAVs is discussed, together with a discussion of a higher level analysis of GAVs and their expected relationships to each other. Gaps in the GAV roster are discussed, with suggestions for estimating the unknown values.

2.2. Group Additivity: A Brief Description

Ever since the efforts of Fajans and Kharasch in the 1920s,[9] there have been numerous efforts to reduce thermochemical properties of organic compounds to a set of bond and group energies. In 1958, Benson and Buss[10] discussed a hierarchy of additivity schemes, and established a conceptual framework that provided a physical justification for the approach.[11] In this hierarchy, atomic additivity is the first level of approximation; the second and third are bond additivity and group additivity, respectively. Atomic additivity (i.e., a particular molecular property can be evaluated as the sum of contributions from the constituent atoms) is valid for such simple properties as molecular weights, but certainly not for thermochemical properties. Bond additivity (i.e., a molecular property is the sum of contributions from each *bond* in the molecule) thus constitutes the first nontrivial level in the Benson and Buss hierarchical scheme, and can often provide useful estimations.

A group is defined by Benson[12] as "a polyvalent atom (ligancy ≥ 2) in a molecule together with all of its ligands." A group is written as $X-(A)_i(B)_j(C)_k(D)_l$, where X is the central atom attached to i A atoms, j B atoms, etc. In the present discussion only C, H, and O atoms are considered, so that X is necessarily a carbon or oxygen atom. Several different types of C atoms are distinguished and notated distinctly: sp^3 (C), sp^2 (C_d), sp (C_t), aromatic sp^2 (C_b), fused ring aromatic (C_{bf}), and allenic carbon, =C= (C_a). C_{bf} can be bonded only to C_b or C_{bf}. C_a is necessarily bonded to two C_d atoms. Two oxygen-containing group families in which the central "atom" is polyatomic are defined: carbonyl (>C=O) and >C=C=O, both of which have two variable ligands.

In addition, there are corrections for nonbonded interactions that are required because of spatial interactions that are not defined in terms of a series of chemical bonds: the most common are the 1,4, or *gauche*, interaction of two methyl groups, and the *cis* and *ortho* interactions. The presence or absence of these corrections depends on interactions of parts of a molecule whose proximity is not implicit in bonding alone. These considerations pose problems for any algorithmic approach to additivity schemes, without which the codification of computer-executable procedures for calculating thermochemical properties would be almost trivial. Other spatial correction terms required are the 1,5 interaction of two substituents such as CH_3, *ene–yne* interactions, and steric hindrance corrections for certain substituted phenanthrenes and naphthalenes. More cumbersome is the fact that most ring structures require unique strain corrections that cannot be derived on the basis of groups themselves. Unfortunately, this enlarges considerably the table of fundamental values that are needed for predicting enthalpies of arbitrary compounds.

One significant effort has been made to extend additivity to the next higher level beyond groups, namely, that of components. However, since the number of required parameters increases rapidly with each hierarchical level, the method of components suffers a series drawback relative the group additivity in spite of its conceptual soundness. The method has been criticized elsewhere.[11]

2.3. Procedure

Once the database was compiled (see Sec. 2.4), GAVs were taken from earlier publications[1,13] and then successively modified to minimize a weighted average error (defined as the experimental value minus the calculated value). This process cannot be described in purely algorithmic terms (as, for example, an unbiased multilinear regression analysis) for several reasons. First, some molecules were given greater weight than others by virtue of their smaller size (hence, fewer different groups involved and smaller cumulative uncertainties), greater number of reported measurements (hence, sometimes, greater accuracy and/or precision), or absence of structural complexities that might invalidate the simplifications inherent in the group additivity method. Because of their unavoidably large experimental uncertainties, very large molecules (say, C_{10}'s and larger) are not particularly useful for deriving GAVs—unless there are no other sources for a particular GAV. Second, values derived for one phase [gas, liquid, or crystal (generally called "solid" in this report)] were taken into consideration in deriving values for another phase. Physically, one would expect GAVs to increase from solid to liquid to gas phase, but the statistical nature of the analysis can lead to small deviations from this order. Large differences in values for different phases—particularly if the gas phase value is larger (i.e., more positive) than liquid, or liquid larger than solid—are taken as a sign of some inconsistencies in the database. Additionally, closely related groups are expected to have similar GAVs, as Table 2 shows. Exceptions to this guideline are generally cases where there is considerable uncertainty in the derived GAVs. Finally, values were recalculated after the omission of a small handful of compounds which, by virtue of particularly large errors, seemed to be experimentally unreliable or else beset with other difficulties.

Molecules with ring structures posed special problems. After all the group contributions to a ringed compound were taken into account (but *not* any corrections for *gauche* or other non-nearest neighbor interactions *within the ring itself*), any remaining disagreement between experimental and calculated enthalpy was assigned to a ring strain correction (RSC) term. To clarify this procedure: if, for example, one were using 3,4-dimethyl-cyclopentadiene to evaluate the RSC for the cyclopentadiene ring, any *cis* or *trans* effects of the methyl side groups would be taken into account, but not any *cis* contributions from the ring members themselves. In many cases, there was only a single compound with the given ring structure, so that there is considerable uncertainty in the assigned RSC.

In the assignment of RSCs for complex structures, one is tempted to try to reduce a ring structure to a sum of its various parts in order to minimize the proliferation of RSC terms. Thus, for example, one might hope to take into account the ring correction in indene by summing the corrections for benzene and cyclopentene; or of triquinacine by a sum of three cyclopentadiene rings. In many cases, such estimations are good to 10–15 kJ/mol, which may not be much larger than experimental uncertainties. However, generally theoretical structure calculations show that the bond angles and lengths in the more complex structures are different from those of the individual ring elements, so there is good reason not to succumb to the temptations of Occam's razor, notwithstanding the benefits that might result from shortening the tables of parameters. All in all, the profusion of RSCs must be regarded, if not as a shortcoming of group additivity, at least as a limiting boundary to its domain of usefulness. Fortunately, there lie well within that boundary such an abundant number of compounds that there is little justice in questioning the method's utility.

2.4. The Database

The database was assembled from several sources, beginning with PNK, which we have found to be an excellent starting point because, unlike many earlier compilations, the authors paid scrupulous attention to which values were indeed the results of measurements and which, on the other hand, were deduced by theory or estimation techniques. (Many of these latter methods are not to be criticized—and certainly have their uses—but in a program aimed at deriving GAVs from the best experimental evidence available, incorporation of values obtained by theory or estimation runs the risk of circularity of argument.) A number of the most complex polycyclic compounds listed in PNK (generally tricyclo- and tetracyclo- species) were omitted because their complex ring geometry, which gave them unique RSCs, made them unlikely to be useful in a generalized estimation program. To the data taken from PNK were added experimental data recorded in several other useful compilations by Stein *et al.*,[7] Lias *et al.*,[14] Domalski and Hearing,[15] and Pedley.[6] References 7 and 14, limited to gas-phase data only, were used selectively, because of the heavy reliance in both on estimated data. SWS includes a tabulation (their Chap. 14) of data for all phases that is annotated as to reliability; data that seemed sufficiently reliable (their category "A" or "B") were incorporated into this database. An important early thermochemical compilation by Kharasch,[16] tabulating experimental heat of combustion data from the 1880s through 1920s, included a pioneering effort to develop simple empirical rules for estimating enthalpies of combustion. Because the reliability of the sources has not been verified (most of them are designated category "C" by SWS), these data (unless they appeared in PNK) have not been incorporated into the database. However, this compendium has been searched to extract a few additional GAVs (highly tentative at present), which are noted in Sec. 2.5 below. A few other sources were also consulted as they became available,[17] but the present database should not be considered as a thorough review of all the published literature.

In general, it has not been possible in this project to evaluate independently the reliability of individual experimental data. Except in a few cases where errors were readily apparent, the experimental data have been accepted as recorded previously.[3,5,6,14,15] One of the best flags to possible experi-

mental errors is a large discrepancy between experimental and calculated values—especially if other, closely related compounds show no such discrepancy.

The database given in this article is partitioned, for convenience of handling, into four Tables. The first, Table 3, lists all C_xH_y compounds; Table 4 lists all C_xH_yO compounds; Table 5 lists $C_xH_yO_2$ compounds, and Table 6, though subtitled $C_xH_yO_3$, includes all compounds with three or more O atoms. The order of listing follows that of PNK: among the C–H compounds, the C subscript is the first determinant, followed by the H subscript, with listings in ascending numerical order. Among the C–H–O compounds, the O subscript is the first determinant, the C subscript is the second, and the H subscript is the last. Following the chemical formula is the parenthetical index assigned by PNK as a bookkeeping convenience. Compounds taken from sources other than PNK (or its successor, Ref. 6) lack such an index. Data for gases, liquids, and solids are tabulated in successive sets of columns. Following the column labeled "Expt" is one labeled "Ref," which is blank if the source was PNK. Other sources are identified by initials or alphabetic references that are cited at the end of each table. The next column lists the enthalpy of formation as calculated by group additivity, using the values of Table 1. The column headed "Δ" gives the discrepancy between experimental and calculated value (Δ=Expt−Calc). It should be noted that we are making no prejudgments whether the difference is a result of experimental inaccuracy, inaccurate GAVs, or breakdown of the assumptions of the GAV method. The four tables include a total of 992 compounds in the gas phase, 935 in the liquid phase, and 590 in the solid phase.

2.5. Format of the Tables

The evaluated GAVs, RSCs, and non-nearest neighbor interactions (NNIs) are listed in Table 1. The first column lists the group, defined in the manner inaugurated by Benson.[1] (Some practitioners have advocated revising this nomenclature, but because the majority of users are familiar with the terminology of Ref. 1, we have chosen not to revise it at this time.) The terms for C–H compounds are listed first, followed by those for C–H–O compounds. For each of the three sets of terms, a column headed "#" lists the number of different compounds in the database in which the pertinent GAV, RSC, or NNI appears. (Multiple occurrences of one GAV in a single compound count as only one appearance.) A "+" sign indicates more than nine compounds. Since GAVs that are derived from only 1, 2, or 3 compounds may be subject to particularly large uncertainties, footnotes to the table identify the compounds used in the evaluation in such cases. These may well signal instances where experimental data ought to be reevaluated or supplemented by measurements on other compounds with the group in question.

As explained in a previous report[18] and noted above, one would expect each liquid phase GAV to be *on average* about 4 kJ/mol (1 kcal/mol) smaller (i.e., less positive) than the corresponding gas phase GAV, and the corresponding solid phase GAV smaller than the liquid GAV by less than 4 kJ/mol. Table 1 shows that these expectations are often borne out, but by no means invariably. We have not ventured to fill in the lacunae in the table by applying this prediction, but in the event that estimations are needed for phases for which some GAVs are lacking, such a procedure would provide a good first guess.

In one special case, a group value has been derived indirectly, rather than from experimental data relating to a molecule that contains the group. This is the case of the $O–(O)_2$ group, derived in detail for the gas phase by Nangia and Benson,[19] but revised in accordance with more recent experimental data.[20]

In most cases, GAVs and RSCs are listed to one significant figure past the decimal point (0.1 or 0.1 kcal/mol). This should not be taken as implying a precision or accuracy of that magnitude; in most cases the uncertainty is considerably greater (2–6 kJ/mol or 0.5–1.5 kcal/mol). In a few cases, particularly with GAVs or RSCs derived from a single experimental datum, the values are listed only to the nearest kJ/mol or kcal/mol; this indicates an uncertainty of several kJ/mol or kcal/mol. In general, though, the number of occurrences of a GAV, RSC, or NNI, rather than the number of significant figures in tabulated entry, is a better indicator of the accuracy of the assigned value.

Ten GAVs in Table 1 are given in brackets. These have been derived from data listed in the compilation by Kharasch.[12] Because the reliability of these experimental studies has not been ascertained, these values must be regarded as tentative at this time, and certainly subject to considerable uncertainty. Because no compounds in Tables 3–6 have these groups, these GAVs have no effect on the calculations in those tables.

Table 1 includes numerical values in both kcal/mol and kJ/mol in successive columns. Because the original data were taken from a variety of sources, it was more convenient to use kcal/mol as the units in which the data manipulations were actually carried out.

Table 2 provides a comparison of the GAVs organized according to group structure. That is, all $C–(\ )(H)_3$ groups, where the empty parentheses can be filled by either C, C_b, C_d, or C_t, are grouped together. The similarities in GAVs for many such groupings is striking, and often reflects the validity of the bond additivity approximation. The use of this table is discussed further in Sec. 2.6 below. Values are given in both kcal/mol and kJ/mol.

All data in Tables 3–6 are in kJ/mol. These tables provide data for C–H, C–H–O, $C–H–O_2$, and $C–H–O_{n>2}$ compounds, respectively. The format is the same. The first column lists compound name, often in more than one form (IUPAC and common names) for the user's convenience. The second column gives the empirical formula, followed by a parenthetical index number that is used by PNK in their compilation. The third column gives the Chem. Abstracts Registry Number, if one has been found. The next four columns pertain to gas phase values, and list, respectively, experimental value, reference, group additivity calculated

value, and the difference between experimental and calculated (experimental-calculated). If there is no entry in the "reference" column, the datum is taken from PNK. In most cases, we accept their evaluation of the best experimental value; in a few cases where we have accepted another value, a footnote indicates the reason. If there is an entry in the references column, it is identified by footnotes at the end of the table. The same set of four entries then follows for liquid and solid (crystal) phases.

It has frequently been the practice to refer to original papers by the keyname used by PNK (or by one of the other secondary compilations upon which we have drawn). Any critical user of these tables will want to have PNK available for reference; therefore we have not felt obliged to repeat their complete journal citations. The extent to which this present work relies on PNK should not be underestimated, though in some instances it has not accepted their recommended evaluations for reasons given in notes.

2.6. Questionable and Undetermined Group Values

As Table 1 shows, in a large number of cases (particularly among the RSCs) there is but a single compound upon whose enthalpy of formation the evaluation rests. There are also many with only two or three sources, often with significant discrepancies among the reported measurements. These instances are footnoted in Table 1. These are all cases for which additional measurements seem essential.

The available GAVs do not exhaust all the possible groups that might occur in organic C–H–O compounds; the arrangement of Table 2 is useful for identifying the 100 or so groups for which experimental data are completely lacking in all three phases. Table 2 also demonstrates that groups with similar structures may have nearly equal GAVs.

For example, although, as noted above, C_b, C_d, C_t, and C are treated as distinct species, it is interesting to compare GAVs for groups that differ only in the nature of the C ligands. In Table 2 there are ten different possible groups of the class $C-(C_x)_2(H)_2$, where the 2 C_x ligands are any combination of C, C_b, C_d, and C_t. For three of these, no GAVs are shown. However, for most of the others the gas phase value is approximately -21 ± 5 kJ/mol; we would therefore expect the missing GAVs to be similar. This rule is true by convention for groups with three H atom ligands (the first group in Table 2); it is quite reliable for groups with two H ligands, and gets progressively poorer for groups with one or no H ligands. This is partly because the number of compounds used to derive the groups with fewer H ligands is smaller, so in general their uncertainties are progressively larger. In fact, the rule does not look very useful for the large number of missing groups of the form $C-(C)_x(C_b)_y(C_d)_z(C_t)_{4-x-y-z}$—carbon atoms with no H atom ligands. The absence of any data for such groups implies their rarity; one is not very likely to require their values in estimating the enthalpy for an unmeasured compound. Thus, if enthalpy estimates are required, it may be possible to estimate an approximate GAV based on the values of similar groups, but this recourse is by no means problem-free.

Can we, from Tables 1 and 2, point to important groups whose values are as yet undetermined in some phase? In a general sense, the answer is no: any group that is relatively important should have already occurred somewhere in the database; its complete absence so far suggests there are not many important compounds that contain it. However, Table 2 does suggest several GAVs that, based on values for other phases or for other similar groups, seem to be in error. Notable among these are: $C-(C_d)_2(H)_2$ (solid; probably in error by 25–30 kJ/mol); $C-(C)(C_d)_2(H)$ (gas and liquid, 5 kJ/mol); $C-(C)_2(C_b)_2$ (liquid and solid; 25–40 kJ/mol); $C-(C)(C_d)(H)(O)$ (liquid; 80 kJ/mol); $C_d-(C_b)(O)$ (solid; 25–40 kJ/mol; $C-(C)_2(C_d)-(O)$ (gas; 60 kJ/mol); and $C-(C_t)(H)_2(CO)$ (solid; 60–100 kJ/mol). Additionally, the various values for $C-(C_x)(H)(O)_2$ for all (C_x) are rather discordant.

Tables 1 and 2 also show numerous instances where there is a large difference in the GAVs for a single group in different phases. These include $C-(C_b)_4$, $C-(C)(C_b)_3$, $C_d-(C_B)(O)$, $C-(C)(C_d)(H)(O)$, and $C-(C)_2(C_B)(O)$. The values reported in this study for the GAVs of these two paragraphs should be regarded as tentative, subject to redetermination.

One group of investigators has proposed redefining some of the groups in fused ring molecules.[21] They define four types of carbon atoms in phenanthrene: $a=C_b-(C_b)_2(H)$, $b=C_b-(C_{bf})(C_b)(H)$, $c=C_{bf}-(C_{bf})(C_b)_2$, and $d=C_{bf}-(C_{bf})_2(C_b)$. In Benson's original treatment, the first two were considered the same $[C_b-(H)]$. We see no need to distinguish b from a for the following reason: b groups will always occur in the presence of c groups; therefore one can only determine $b+c$ experimentally. Thus we are free to set $b=a$ by definition. However, this does raise the question whether one should treat the nine and ten carbons in anthracene (call them e for now) as different from ordinary C_b atoms, inasmuch as they are bonded to two c-type C atoms. This is possible, and the fact that the calculated enthalpy for anthracene differs from the experimental by 15 kJ/mol on the assumption that $e=b=a$ suggests that perhaps e has a different value. The objection to this argument is that the present GAVs do fit naphthacene quite well (i.e., suggesting e does equal b and a). Hence, there is no current basis for defining e groups differently until the discrepancy between anthracene and naphthacene enthalpies can be resolved.

2.7. Non-Nearest Neighbor Interactions

Another area in which data are insufficient to draw definitive conclusions is that of non-nearest neighbor interactions; e.g., *cis*, *ortho*, and *gauche* effects, which involve atoms separated by at least two other atoms (normal group additivity relations take into account interactions between atoms with at most one atom between them). Table 1 lists 21 such correction terms, but in many cases they rest on inconclusive

or even contradictory data. For example, consider the enthalpies of formation for the following compounds with 1,2-substitutions on a five-carbon ring in the solid phase (all enthalpies are in kJ/mol):

Compound	*Cis* (*Z*)	*Trans* (*E*)	(*E*)−(Z)
1,2-indanylene diacetate	−774.5	−759.8	15.3
1,2-cyclopentylene dibenzoate	−667.3	−674.9	−7.6
1,2-indanylene dibenzoate	−555.2	−546.8	5.4

If these data are reliable, the two adjacent –C(O)O– groups in the (*Z*) configuration are less stable in one pair, but more stable in two pairs, though one would in general expect less stability. (The difference in the indanylene rings owing to the presence of an attached aromatic ring should have slight effect on this comparison.)

Or consider the following trimethyl benzoic acids in solid phase, all measured in the same study:

Compound	Enthalpy kJ/mol	Number of adjacent groups CH_3–CH_3	Number of adjacent groups CH_3–COOH
2,3,4-TMB	−487	2	1
2,3,5-TMB	−489	1	1
2,3,6-TMB	−476	1	2
2,4,5-TMB	−496	1	1
2,4,6-TMB	−478	0	2
3,4,5-TMB	−501	2	0

Comparing 2,3,6 with 2,4,5, it appears that adding a CH_3–COOH neighbor to one neighboring CH_3 pair destabilizes by 20 kJ/mol; adding it to two neighboring CH_3 pairs (compare 2,3,4 with 3,4,5) decreases stability by 14 kJ/mol. And two compounds with the same apparent number of *ortho* effects (2,3,5 and 2,4,5) differ by 7 kJ/mol—either a measure of the imprecision of the data or of the presence of some other, more subtle effects.

It is conceptually appealing to try to resolve these difficulties by introducing a nonadditive hindrance correction such as buttress effect—an additional strain present when three or more adjacent substituents are present.[22] But the experimental data at hand do not provide consistent justification for such an effect. For example, consider the data for the benzene tri- tetra-, penta-, and hexacarboxylic acids in the solid phase. If there are buttressing effects, one would expect the error, when the calculations take into account only standard groups and additive *ortho* corrections, to increase with increasing number of carboxy groups. The data on the last page of Table 6 do not support this prediction. Below, the second column lists for each of these compounds the experimental enthalpy minus the ordinary group contributions. The difference should represent any *ortho* and buttressing corrections. The third column is the remainder after subtracting a correction of 25.5 kJ/mol (from Table 1 for each carboxy–carboxy *ortho* interaction).

Compound	Expt−GAVs	Expt−GAV−Ortho
1,2,3-tricarboxylic acid	46	−4
1,2,4-tricarboxylic acid	28	3
1,3,5-tricarboxylic acid	18	18
1,2,3,4-tetracarboxylic acid	73	−3
1,2,3,5-tetracarboxylic acid	59	9
1,2,4,5-tetracarboxylic acid	51	1
Pentacarboxylic acid	106	6
Hexacarboxylic acid	152	1

The one molecule with significant error is the 1,3,5-tricarboxylic acid, for which there should be no *ortho* or buttressing effects. Since the GAVs are determined by a much larger database than just these eight compounds, it is difficult to argue that changing the GAVs will reveal the presence of buttressing effects. (Note also that the data do not support the existence of a consistent negative *meta* contribution, as has been proposed in other estimation schemes.)

As a final example, consider the dimethoxy-substituted benzene and benzoic acid in the gas phase. According to Table 1, the *ortho* correction for methoxy adjacent to COOH is the same as for two adjacent methoxy groups,

Compound	Expt−GAVs	Expt−GAVs−Ortho
2,3-dimethoxybenzoic acid	31	6
2,6-dimethoxybenzoic acid	29	4
3,4-dimethoxybenzoic acid	17	5
2,4-dimethoxybenzoic acid	13	0
3,5-dimethoxybenzoic acid	4	4
1,2-dimethoxybenzene	−7	−19

Again, no buttressing effect is apparent (it should show up in the 2,3-, and 2,6-dimethoxybenzoic acids and not others). (Note also that the dimethoxybenzene, unlike the other compounds, shows no evidence for *ortho* destabilization by the methoxy groups.) Similar conclusions result from data for the tri- tetra-, penta- and hexamethyl benzenes; no unambiguous non-additive corrections were evident.

Other steric effects present similar problems resulting from inadequate or inconsistent data. Consider next the ether *gauche* effect (the 1–4 interaction across an O atom bridging two alkyl groups). In Ref. 1, a value of 2.1 kJ/mol (0.5 kcal/mol) was recommended. Reanalysis of the best currently available data suggests that 3.3 kJ/mol (0.8 kcal/mol) is a better value, though, as the table below comparing the differences between experimental and calculated enthalpies (with a 3.3 kJ/mol *gauche* correction) shows, there is considerable scatter in the data. The second column, labeled "G," is the number of *gauche* interactions.

Compound	G	Expt−Calc
Methyl isopropyl ether	1	0
Methyl t-butyl ether	2	4
Isopropyl isopropyl ether	2	1
Isopropyl t-butyl ether	3	−1
Ethyl s-butyl ether	1	−7
s-butyl s-butyl ether	2	1

With the present value of 3.3 kJ/mol destablization for each *gauche* interaction, the "*ether gauche*" effect is no different from the ordinary alkyl *gauche* effect. However, we have tabulated them separately to facilitate later reevaluation. (In principle, the *gauche* effect across a carbonyl group could have a different value, but again, within the scatter of the data, 3.3 kJ/mol seems to be the best choice, and we have not distinguished this interaction from an ordinary *gauche* interaction.)

Another possible non-nearest neighbor interaction that has been suggested is hydrogen bonding between vicinal OH groups in diols.[23] Several polyols for which gas or liquid phase data are available are shown below. The last column headed "*V*" gives the number of neighboring OH groups.

	Expt−Calc		
Compound	Gas	Liquid	*V*
1,2-ethanediol	−2.5	−1.7	1
1,2-propanediol	1.7	10.9	1
1,3-propanediol	13.8	17.6	0
1,2-butanediol		−1.7	1
1,3-butanediol	10.9	20.9	0
2,3-butanediol	−21.3	−5.4	1
1,2,3-propanetriol	−9.1	7.9	2
1,2,3,4-butanetetrol	−13.0	9.2	3

Taken at face value, the data suggest possibly some stabilization effect in the gas, but probably less in the liquid. A hydrogen bond of 8–16 kJ/mol is not unreasonable; but the magnitude of the effect is clearly not constant. Because of the overall inconsistency between calculated and experimental values, without evidence of a consistent effect, no correction term is recommended until the experimental numbers can be corroborated.

2.8. Summary and Conclusions

This compilation takes its place in the literature alongside several others, cited earlier, each of which offers some of its own advantages. The distinctive features of the present work are: (1) an extension and revision of Benson's group additivity method, the procedure that seems to have the most widespread acceptance at present, and the overall best record for reliability of estimation techniques; (2) a strict reliance on experimental values as basis for evaluating group additivity parameters; (3) a simultaneous compilation and evaluation of data for all three phases—gas, liquid, solid—thereby giving an additional basis for comparison of reliabilities; (4) an unambiguous procedure for extending the groups to compounds containing other than only carbon, hydrogen, and oxygen, thus permitting the extension of the present database and table of group additivity parameters to many more compounds.

A total of 54 C–H and 111 C–H–O groups were found in the course of this evaluation, as well as 200 ring strain correction factors and 21 non-nearest neighbor interactions. Not all of these have been evaluated in all three phases. Of them, the gas phase lacks 22 GAVs, 31 RSCs, and 1 NNI. This represents a considerable increase over Ref. 1 (Table A2), in which are tabulated 98 GAVs and 68 RSCs in the gas phase. A new family of groups (>C=C=O), analogous to the carbonyl groups (C=O), has been defined. Also, some new non-nearest-neighbor corrections have been identified: The ditertiary ketone steric correction is similar to the ditertiary ether correction. Like the latter, it occurs in a single compound so far. Some specific *cis*, *gauche*, and *ortho* corrections have also been tentatively identified.

The group additivity values and ring strain correction terms derived in this study predict quite well the enthalpies of formation of most of the compounds in the database. In the gas phase, for which agreement is best, the average error for 1028 compounds (17, for which discrepancies were very large—greater than 42 kJ/mol—were excluded) was approximately 5.5 kJ/mol (1.32 kcal/mol). For the liquid phase, the average error for the 941 compounds retained out of 971 total was 5.6 kJ/mol (1.34 kcal/mol). For the solid phase, the average error for the 538 kept out of 584 total was 9.1 kJ/mol (2.17 kcal/mol).[24] The average error in the gas phase database is probably no larger than the average experimental uncertainty, and is as good as one could expect. The solid phase database shows some room for improvement, but the defects may well reside in the experimental uncertainties. Alternatively, it is possible that intermolecular forces in condensed phases, which often lie outside the conceptual framework of group additivity, contribute at least in some cases to the larger discrepancies between calculated and experimental enthalpies. A comparison of the average discrepancies in the different phases suggests that if intermolecular forces do limit the utility of group additivity in condensed phases, they are significantly only in the solid, and not in the liquid phase.

Table 2 shows there are numerous groups as yet completely undetermined, but, as discussed in Sec. 2.6, probably none is greatly important. However, the discrepancy in the enthalpies of anthracene and naphthacene is of some significance, because it holds the answer to whether the 9 and 10 carbons of the anthracene molecule (and similar aromatic carbon atoms) need to be treated as distinct from the other C_b atoms. The discussion of Sec. 2.7 concludes that many non-nearest neighbor interactions are subject to great experimental uncertainty that might benefit from a series of carefully conducted measurements.

It is possible that a few ambiguities and uncertainties will be clarified if this project continues through other groups of compounds: carbon–hydrogen–oxygen–nitrogen, etc.

3. Tables of C–H–O Compounds

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 1

Group (C-H)	Gas GAV			Liquid GAV			Solid GAV			Notes
	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	
C-(C)(H)3	-10.0	-41.8	+	-11.6	-48.5	+	-10.1	-42.3	+	
C-(C)2(H)2	-5.0	-20.9	+	-6.1	-25.5	+	-7.0	-29.3	+	
C-(C)3(H)	-2.4	-10.0	+	-2.2	-9.2	+	-4.0	-16.7	+	
C-(C)4	-0.1	-0.4	+	0.8	3.3	+	-1.5	-6.3	+	
Cd-(H)2	6.3	26.4	+	4.9	20.5	+	6.0	25.1	+	
Cd-(C)(H)	8.6	36.0	+	7.7	32.2	+	6.1	25.5	+	
Cd-(C)2	10.2	42.7	+	9.7	40.6	+				
Cd-(Cd)(H)	6.8	28.5	+	5.3	22.2	+	5.2	21.8	+	
Cd-(C)(Cd)	8.8	36.8	6	8.0	33.5	8	7.7	32.2	2	1
Cd-(Cd)2	6.6	27.6	7	4.0	16.7	1	2.7	11.3	3	2
C-(Cd)(H)3	-10.0	-41.8	+	-11.6	-48.5	+	-10.1	-42.3	+	3
C-(C)(Cd)(H)2	-4.8	-20.1	+	-6.1	-25.5	+	-5.0	-20.9	5	
C-(C)2(Cd)(H)	-1.7	-7.1	+	-2.4	-10.0	+	-3.0	-12.6	5	
C-(C)3(Cd)	1.7	7.1	+	2.3	9.6	+	4.3	18.0	1	4
C-(Cd)2(H)2	-4.3	-18.0	9	-5.8	-24.3	5	-13.3	-55.6	1	5
C-(C)(Cd)2(H)	2.7	11.3	3	1.8	7.5	1				6
C-(C)2(Cd)2	6.8	28.5	1	5.2	21.8	1				7
Allyl [>C=C=C<]	34.2	143.1	5	32.7	136.8	3				8
Ct-(H)	27.2	113.8	+	26.0	108.8	+				
Ct-(C)	27.3	114.2	+	25.5	106.7	+	23.9	100.0	+	
Ct-(Ct)	25.3	105.9	3	25.2	105.4	1	24.7	103.3	2	9
C-(Ct)(H)3	-10	-41.8	+	-11.6	-48.5	+	-10.1	-42.3	+	10
C-(C)(Ct)(H)2	-4.7	-19.7	+	-5.3	-22.2	+	-7.1	-29.7	1	11
C-(C)2(Ct)(H)	-1.8	-7.5	6	-2.0	-8.4	6				
C-(C)3(Ct)	1.3	5.4	4	1.9	7.9	2	0.5	2.1	1	12
C-(C)2(Ct)2				3.5	14.6	1				13
Cd-(Ct)(H)	6.7	28.0	6	4.7	19.7	5				
Cd-(C)(Ct)	9.5	39.7	2							14
Ct-(Cd)	27.9	116.7	8	28.0	117.2	5				
Cb-(H)	3.3	13.8	+	2.0	8.2	+	1.5	6.3	+	
Cb-(C)	5.5	23.0	+	4.8	20.1	+	2.9	12.1	+	
C-(Cb)(H)3	-10	-41.8	+	-11.6	-48.5	+	-10.1	-42.3	+	15
C-(C)(Cb)(H)2	-4.6	-19.2	+	-6.2	-25.9	+	-6.5	-27.2	+	
C-(C)2(Cb)(H)	-1	-4.2	+	-1.0	-4.2	+	-1.0	-4.2	+	
C-(C)3(Cb)	2.9	12.1	+	3.4	14.2	+	0.4	1.7	+	
C-(Cb)2(H)2	-6.3	-26.4	4	-5.2	-21.8	5	-6.0	-25.1	4	
C-(C)(Cb)2(H)	-1.1	-4.6	1	6.5	27.2	3	5.6	23.4	7	16
C-(C)2(Cb)2				[10]	[42]		9.8	41.0	1	17
C-(Cb)3(H)	-1	-4.2	2				9.8	41.0	2	18
C-(C)(Cb)3	4.3	18.0	1				30.0	125.5	4	19
C-(Cb)4	7.3	30.5	1				17.5	73.2	1	20
Cb-(Cd)	5.8	24.3	9	8.0	33.5	+	5.8	24.3	+	
Cb-(Ct)	5.7	23.8	4	5.5	23.0	1	5.5	23.0	4	21
Cb-(Cb)	5.2	21.8	8	5.0	20.9	4	4.4	18.4	+	
Cd-(Cb)(H)	6.8	28.5	8	1.5	6.3	8	3.0	12.6	+	
Cd-(C)(Cb)				5.7	23.8	2	5.0	20.9	1	22
Cd-(Cb)2	8	33.5	2	7.2	30.1	1	9.6	40.2	9	23
Cd-(Cb)(Cd)	13	54.4	2				13.2	55.2	4	24
Ct-(Cb)	24.6	102.9	4	26.5	110.9	1	23.5	98.3	4	25
C-(Cb)(Cd)(H)2	-2.5	-10.5	1	-4.7	-19.7	2				26
C-(C)(Cb)(Cd)(H)				-2.1	-8.8	1				27
Cbf-(Cbf)(Cb)2	4.7	19.7	+	3.3	13.8	4	4.2	17.6	+	
Cbf-(Cbf)2(Cb)	4.4	18.4	+				2.9	12.1	+	
Cbf-(Cbf)3	2.4	10.0	2				0.9	3.8	2	28

Bracketed values are estimates, generally subject to uncertainties of more than 8-12 kJ/mol (2-3 kcal/mol).

#: These columns indicate the total number of compounds in the databases with the indicated group. "+" means >9 compounds.

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 2

Ring strain corrections (C-H)	Gas RSC			Liquid RSC			Solid RSC			Notes
	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	
Cyclopropane	27.7	115.9	7	27.0	113.0	+				
Cyclopropene	53.6	224.3	2							29
Methylenecyclopropane	41	171.5	1	8.2	34.3	1				30
Cyclobutane	26.8	112.1	5	25.3	105.9	7				
Methylenecyclobutane	27.2	113.8	1	26.0	108.8	1				31
Cyclobutene	29.8	124.7	2				29.6	123.8	1	32
Cyclopentane	7.1	29.7	+	5.4	22.6	+				33
Cyclopentene	5.9	24.7	+	4.7	19.7	5	2.2	9.2	2	34
Cyclopentadiene	5.7	23.8	1	5.2	21.8	1				35
Cyclohexane	0.7	2.9	+	-0.7	-2.9	+	0.0	0.0	6	
Cyclohexene	0.5	2.1	7	-0.8	-3.3	+				
Cyclohexadiene (1,3)	4	16.7	5	4.0	16.7	3				36
Cyclohexadiene (1,4)	-3.0	-12.6	3	-3.4	-14.2	1				37
3-Methylene-cyclohexene				-9.0	-37.7	1				38
Cycloheptane	6.8	28.5	2	5.3	22.2	5				39
Cycloheptene	5.4	22.6	1							40
Cycloheptadiene (1,3)	6.5	27.2	1	4.9	20.5	1				41
Cycloheptadiene (1,4)				5.9	24.7	1				42
Cycloheptatriene	3.4	14.2	1	3.3	13.8	1	0.0	0.0	1	43
Cyclooctane	10.3	43.1	1	8.8	36.8	1				44
Cyclooctene (Z)	6	25.1	1	3.6	15.1	1				45
Cyclooctene (E)				13.5	56.5	1				46
Cyclooctadiene (Z-Z-1,5)	9	37.7	1	7.6	31.8	1				47
Cyclooctatetraene	16.5	69.0	1	18.4	77.0	1				48
Cyclononane	13.3	55.6	1	11.7	49.0	1				49
Cyclononene (Z)				7.8	32.6	1				50
Cyclononene (E)				10.6	44.4	1				51
Cyclononatriene (1,4,7)				5.0	20.9	1				52
Cyclodecane	13.1	54.8	1	11.7	49.0	3				53
Cyclodecene (Z)				4.8	20.1	1				54
Cyclodecene (E)				8.2	34.3	1				55
Cycloundecane	12.1	50.6	1	10.9	45.6	1				56
Cyclododecane	5	20.9	1				11.0	46.0	1	57
Cyclododecatriene (E,E,Z,1,5,9)	0.6	2.5	1	-2.1	-8.8	1				58
Cyclododecatriene (E,E,E,1,5,9)	1.7	7.1	1				0.0	0.0	1	59
Cyclotridecane	6.1	25.5	1	5.4	22.6	1				60
Cyclotetradecane	5.8	24.3	1				8.6	36.0	1	61
Cyclotetradecadiyne (1,8)	14.9	62.3	1				10.0	41.8	1	62
Cyclopentadecane	3	12.6	1				15.0	62.8	1	63
Cyclohexadecane	3	12.6	1				15.6	65.3	1	64
Cyclohexadecaoctaene (16-Annulene)							48.0	200.8	1	65
Cycloheptadecane	-2.1	-8.8	1				16.0	66.9	1	66
Cyclooctadecanonaene (18-Annulene)							2.4	10.0	1	67
Cyclotriacontane							0.0	0.0	1	65
Bicyclo-[1.1.0]-butane	67	280.3	1	62.0	259.4	2	62.0	259.4	1	66
Bicyclo-[2.1.0]-pentane				55.0	230.1	1				67
Bicyclo-[3.1.0]-hexane	33.4	139.7	2	29.8	124.7	2				68
Bicyclo-[2.2.1]-hexene				56.1	234.7	1				69

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 3

Ring strain corrections (C-H)	Gas RSC			Liquid RSC			Solid RSC			Notes
	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	
Bicyclo-[4.1.0]-heptane	30.2	126.4	4	26.2	109.6	4				
Bicyclo-[3.1.1]-heptane; ene	30.6	128.0	2	27.1	113.4	2				70
Bicyclo-[3.2.0]-hept-2-ene	36.6	153.1	1							71
Norbornane (Bicyclo-[2.2.1]-heptane)	16	66.9	8	16.0	66.9	+	20.0	83.7	4	
Norbornene	22.8	95.4	2				27.5	115.1	2	72
Bicyclo-[5.1.0]-octane	30.8	128.9	1	26.7	111.7	1				73
Bicyclo-[4.2.0]-octane	28.5	119.2	1	24.8	103.8	1				74
Bicyclo-[2.2.2]-octane; -ene	10.6	44.4	4	8.0	33.5	4	16.3	68.2	1	75
(Z)-Bicyclo[3.3.0]octane (Octahydropentalene)	10.2	42.7	1	6.8	28.5	1				76
(E)-Bicyclo[3.3.0]octane	16.5	69.0	1	13.3	55.6	1				77
Bicyclo-[6.1.0]-nonane	30.8	128.9	2	27.2	113.8	2				78
Bicyclo-[3.3.1]-nonane	9.3	38.9	1				14.5	60.7	1	79
Bicyclo-[3.3.1]-2-nonene	8.4	35.1	1				11.8	49.4	1	80
Bicyclo-[3.2.2]-6-nonene	10.4	43.5	1				16.5	69.0	1	81
Bicyclo-[4.2.1]-3-nonene	13.1	54.8	1				15.9	66.5	1	82
Bicyclo-[3.3.2]-decane	19.4	81.2	1				24.8	103.8	1	83
Bicyclo-[5.3.0]-decane	13.5	56.5	1	9.3	38.9	1				84
Tetracyclo[5.2.1.0^2,6]decane	29.8	124.7	1				28.5	119.2	1	85
Tetracyclo[5.2.1.0^2,6.0^3,5]-8-decene				70.8	296.2	1				86
Bicyclo-[3.3.3]-undecane	28.5	119.2	1				34.6	144.8	1	87
Bicyclo-[4.4.1]-undecane	7.8	32.6	1	8.1	33.9	1				88
Indane	4.6	19.2	5	3.8	15.9	5	5.8	24.3	7	
Indene	1.7	7.1	1	1.3	5.4	1				89
Methanoindene	25.3	105.9	1	19.1	79.9	1	27.0	113.0	2	90
Cyclobutylbenzene	33.1	138.5	1							91
Cyclopropylbenzene	70.7	295.8	2							92
1,2-Dihydronaphthalene	-2.4	-10.0	1	-0.4	-1.7	1				93
1,4-Dihydronaphthalene				-11.1	-46.4	1				94
Biphenylene	52.6	220.1	1				50.3	210.5	1	95
Spiropentane	64.4	269.4	1	61.4	256.9	1				96
Fulvene	10	41.8	3	7.0	29.3	1	8.6	36.0	1	97
Azulene	1.6	6.7	1				3.6	15.1	2	98
Adamantane	7.4	31.0	7				11.7	49.0	7	
Diamantane	16	66.9	7	3.6	15.1	1	19	79.5	7	99
Fluoranthene	6	25.1	1				4.5	18.8	1	100
Acenaphthene	6.5	27.2	1				6.7	28.0	1	101
Triquinacine	7	29.3	3							102
Perhydroquinacine	15.1	63.2	1				20.0	83.7	1	103
Dodecahydrotriphenylene							17.3	72.4	1	104
1,4[1',2']-Benzenocyclohexane	6.3	26.4	1				-3.1	-13.0	1	105
9,10-Dihydroanthracene	2.2	9.2	2				3.5	14.6	2	106
9,10-Dihydrophenanthrene				-10.5	-43.9	1				107
Octahydroanthracene	0.9	3.8	1	1.8	7.5	1	10.8	45.2	1	108
1,2,3,4-Tetrahydronaphthalene	1.2	5.0	1	0.2	0.8	1	-2.0	-8.4	2	109

Non-nearest neighbor interactions (C-H)	Gas Correction			Liquid Correction			Solid Correction			Notes
	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	
Alkane gauche correction	0.8	3.3	+	0.6	2.3	+	0.4	1.7	7	
1-5 Correction	1.6	6.7	+	2.1	8.7	+	3.1	13.0	2	110
Cis correction	1.1	4.6	+	0.9	3.8	+	1.0	4.2	+	
Cis correction (1 t-Bu)	4.4	18.4	4	3.6	15.1	4				
Cis correction (2 t-Bu)				10.3	43.1	1				111
2 Cis corrections about same bond	3.3	13.8	1	2.7	11.3	2	2.7	11.3	1	112
Alkene gauche correction	0.8	3.3	5	1.0	4.2	7				
Ene-yne cis correction	-0.7	-2.9	2	-0.6	-2.5	2				113
Ortho correction (also cis on C5 rings)	0.6	2.5	+	0.4	1.7	+	0.6	2.5	+	
Ortho (2 t-butyls)	20.8	87.0	1				17.1	71.5	2	114
Phenanthrene 4-5 correction	10.5	43.9	6				10.0	41.8	7	115
Naphthalene 1-8 correction	5.3	22.2	5	6.5	27.2	2	5.0	20.9	5	116

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 4

Group (C-H-O)	Gas GAV			Liquid GAV			Solid GAV			Notes
	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	
O-(H)2	-57.8	-241.8	1	-68.3	-285.8	1	-69.7	-291.8	1	117
O-(C)(H)	-37.9	-158.6	+	-45.5	-190.4	+	-50.0	-209.2	+	
O-(Cb)(H)	-38.5	-161.1	+	-46.6	-195.0	+	-46.7	-195.4	+	
O-(Cd)(H)	-49.3	-206.3	+	-51	-213.4	5	-52.4	-219.2	4	
O-(Ct)(H)	[37.9]	[158.6]								118
O-(H)(CO)	-57.8	-241.8	+	-66.2	-277.0	+	-61.4	-256.9	+	
O-(C)2	-23.8	-99.6	+	-25.1	-105.0	+	-25.0	-104.6	+	
O-(C)(Cb)	-21.6	-90.4	+	-25.0	-104.6	9	-32.2	-134.7	6	
O-(C)(Cd)	-30.5	-127.6	+	-31.0	-129.7	+	-31.0	-129.7	1	119
O-(C)(CO)	-43.1	-180.3	+	-44.5	-186.2	+	-44.0	-184.1	+	
O-(Cb)2	-18.9	-79.1	4	-20.4	-85.4	1	-19.0	-79.5	4	120
O-(Cb)(Cd)	-21	-87.9	4	-26.6	-111.3	1				121
O-(Cd)2	-33	-138.1	+	-33.0	-138.1	8	-33.0	-138.1	7	
O-(Cb)(CO)	-36.7	-153.6	7	-37.0	-154.8	5	-35.0	-146.4	9	
O-(Cd)(CO)	-44.8	-187.4	2	-45.0	-188.3	3				122
O-(CO)2	-46.2	-193.3	+	-53.0	-221.8	+	-51.0	-213.4	+	
O-(H)(O)	-16.3	-68.2	4	-22.8	-95.4	+	-23.9	-100.2	+	123
O-(C)(O)	-5	-20.9	+	-6.2	-25.9	+	-11.0	-46.0	5	124
O-(Cb)(O)	[-5]	[-21]	0				-4.5	-18.8	1	125
O-(O)(CO)	-18.2	-76.1	4	-20.8	-87.0	8	-15.4	-64.4	+	126
O-(O)2	14.7	61.5		[13.4]	[56.1]					127
C-(H)3(O)	-10	-41.8		-11.6	-48.5		-10.1	-42.3		128
C-(H)2(O)2	-16.5	-69.0	+	-16.6	-69.5	+	-18.5	-77.4	4	
C-(C)(H)2(O)	-8.1	-33.9	+	-9.1	-38.1	+	-5.0	-20.9	+	
C-(C)2(H)(O)	-7.2	-30.1	+	-7.0	-29.3	+	-1.0	-4.2	+	
C-(C)(H)(O)2	-15.8	-66.1	+	-16.0	-66.9	+	-20.0	-83.7	+	
C-(C)3(O)	-6.6	-27.6	+	-5.6	-23.4	+	-5.6	-23.4	9	
C-(C)2(O)2	-16.2	-67.8	3	-15.8	-66.1	+				129
C-(C)(O)3	-25.5	-106.7	1	-24.7	-103.3	1				130
C-(H)(O)3	-26.8	-112.1	2	-25.3	-105.9	2				131
C-(O)4	-38.6	-161.5	2	-36.7	-153.6	2				132
C-(Cd)(H)2(O)	-6.9	-28.9	5	-8.0	-33.5	3				133
C-(Cd)(H)(O)2	-0.3	-1.3	1				-7.0	-29.3	1	134
C-(C)2(Cd)(O)	13	54.4	2							135
C-(C)(Cd)(H)(O)				-29.2	-122.2	3	-5.0	-20.9	3	136
C-(C)2(Ct)(O)							1.5	6.3	2	137
C-(Ct)(H)2(O)	-8.6	-36.0	1	[-6]	[25]					138
C-(Ct)(H)2(CO)	-5	-20.9	1	-4.9	-20.5	1	15.2	63.6	1	139
C-(Ct)(O)3							28.4	118.8	1	140
C-(Cb)(H)2(O)	-12.4	-51.9	2				-3.0	-12.6	2	141
C-(Cb)(H)(O)2							0.1	0.4	1	142
C-(Cb)2(H)(O)							-1.0	-4.2	1	143
C-(Cb)(H)2(CO)	-5.4	-22.6	4	-3.1	-13.0	1	-3.0	-12.6	7	144
C-(Cb)(H)(O)(CO)							7.9	33.1	1	145
C-(C)(Cb)(H)(O)	-4.4	-18.4	2				0.1	0.4	7	146
C-(C)2(Cb)(O)	-4.2	-17.6	2	1.8	7.5	1	17.9	74.9	2	147
C-(Cb)2(O)2							54.0	225.9	1	148
C-(Cb)3(O)							18.0	75.3	4	149
C-(C)(Cb)(Cd)(O)	-4.7	-19.7	1				7.2	30.1	1	150
C-(Cb)(Cd)(H)(O)	-4.8	-20.1	1							151
C-(Cb)2(Cd)(O)							-2.0	-8.4	1	152
C-(H)2(O)(CO)							-4.6	-19.2	1	153
C-(C)(H)2(CO)	-5.2	-21.8	+	-5.2	-21.8	+	-14.6	-61.1	+	
C-(C)2(H)(CO)	-1.7	-7.1	+	-1.4	-5.9	+	-9.0	-37.7	+	
C-(C)3(CO)	1.4	5.9	+	3.5	14.6	9	-5.2	-21.8	+	
C-(H)2(CO)2	-6.6	-27.6	5	-5.8	-24.3	5	-8.0	-33.5	4	154
C-(C)(H)(CO)2							-14.0	-58.6	+	

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 5

Group (C-H-O)	Gas GAV			Liquid GAV			Solid GAV			Notes
	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	
C-(H)3(CO)	-10	-41.8		11.6	48.5		-10.1	-42.3		155
C-(C)2(CO)2	1.6	6.7	1				10.3	43.1	1	156
C-(C)(H)(O)(CO)	-4.5	-18.8	1				-6.9	-28.9	2	157
C-(Cd)(H)(O)(CO)							[10]	[40]		158
C-(C)2(O)(CO)							13.5	56.5	3	159
C-(O)2(CO)2							[3]	[12]		160
C-(C)(Cb)(H)(CO)							1.0	4.2	4	
C-(Cd)(H)2(CO)	-3.8	-15.9	7	-8.0	-33.5	6	-15.0	-62.8	3	161
C-(Cb)2(Ct)(O)				[2.5]	[10]					162
C-(H)(CO)3				[-11]	[-46]					163
C-(H)(O)(CO)2							[-9.5]	[-40]		164
CO-(C)(H)	-29.4	-123.0	+	-34.3	-143.5	7				
CO-(H)(O)	-31.9	-133.5	3	-36.2	-151.5	3				165
CO-(H)(CO)	-25.2	-105.4	2	-32.3	-135.1	1	-41.0	-171.5	1	166
CO-(C)2	-31.7	-132.6	+	-36.2	-151.5	+	-35.4	-148.1	+	
CO-(C)(O)	-35.2	-147.3	+	-38.1	-159.4	+	-35.5	-148.5	+	
CO-(C)(CO)	-30.2	-126.4	4	-32.1	-134.3	2	-21.8	-91.2	1	167
CO-(O)2	-29.9	-125.1	9	-30.0	-125.5	5	-33.0	-138.1	5	
CO-(O)(CO)	-29.5	-123.4	5	-31.7	-132.6	3	-36.0	-150.6	5	168
CO-(C)(Cd)	-32.4	-135.6	+	-32.0	-133.9	4	-27.0	-113.0	4	169
CO-(Cd)(H)	-27.6	-115.5	8	-30.0	-125.5	3	-35.1	-146.9	1	170
CO-(Cd)2	-30	-125.5	7	-31.0	-129.7	1	-39.0	-163.2	8	171
CO-(Cd)(O)	-32.2	-134.7	+	-32.7	-136.8	+	-39.0	-163.2	+	
CO-(Ct)(O)	-39.5	-165.3	1	-35.2	-147.3	3	-34.1	-142.7	2	172
CO-(Cb)(H)	-29.1	-121.8	2	-35.0	-146.4	3	-29.8	-124.7	2	173
CO-(C)(Cb)	-30.9	-129.3	7	-37.0	-154.8	7	-39.5	-165.3	+	
CO-(Cb)2	-27	-113.0	9	-28.0	-117.2	3	-33.5	-140.2	9	174
CO-(Cb)(O)	-34.4	-143.9	+	-36.9	-154.4	+	-40.8	-170.7	+	
CO-(Cb)(CO)	-26.5	-110.9	2				-30.4	-127.2	2	175
CO-(Cb)(Cd)	-39.8	-166.5	2				-31.9	-133.5	3	176
CO-(Cd)(CO)	-28.3	-118.4	1	-28.1	-117.6	1	-28.0	-117.2	1	177
CO-(C)(Ct)	-30	-125.5	1	[-42]	[-176]					178
Cd-(H)(CO)	5.2	21.8	+	2.0	8.4	+	6.0	25.1	+	
Cd-(C)(O)	8.9	37.2	+	5.0	20.9	7	4.0	16.7	2	179
Cd-(H)(O)	8.6	36.0	+	7.0	29.3	+	0.0	0.0	6	
Cd-(Cd)(O)	9.5	39.7	6	9.0	37.7	3	9.0	37.7	4	180
Cd-(C)(CO)	7.5	31.4	9	9.8	41.0	4	7.8	32.6	8	
Cd-(O)(CO)	11.6	48.5	5	6.0	25.1	3	8.0	33.5	5	181
Cd-(Cb)(O)	10.4	43.5	4				1.2	5.0	1	182
Cd-(Cb)(CO)	8	33.5	1				8.0	33.5	1	183
Cd-(Cd)(CO)	8.3	34.7	2	1.9	7.9	1				184
Cd-(CO)2	13.3	55.6	1				[27]	[113]		185
Cd-(Ct)(O)	7.6	31.8	1							186
Cb-(O)	-0.9	-3.8	+	-1.4	-5.9	+	-1.0	-4.2	+	
Cb-(CO)	3.7	15.5	+	4.2	17.6	+	4.5	18.8	+	
CCO-(H)2	-11.4	-47.7	1	-16.2	-67.8	1				187
CCO-(C)(H)	-15	-62.8	1							188
CCO-(C)2	-12	-50.2	1							189
CCO-(Cb)(H)	-25.6	-107.1	1							190
CCO-(Cb)2	-15.8	-66.1	1							191
C-(CCO)(H)3	-10	-41.8	2	-11.6	-48.5	0	-10.1	-42.3	0	192
Cb-(CCO)	4	16.7	2							193
Ct-(O)	[31.9]	[133.5]								194
Ct-(CO)	28.4	118.8	2	29.0	121.3	3	25.6	107.1	1	195

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 6

Non-nearest neighbor interactions (C-H-O)	Gas Correction			Liquid Correction			Solid Correction			Notes
	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	
Ether gauche	0.8	3.3	+	0.7	2.9	+				
Oxygen gauche	0.0	0.0	+	0.0	0.0	+	0.0	0.0	+	
Ditertiary ether	10.5	43.9	1	10.1	42.3	1				196
Ditertiary ketone	6.3	26.4	1	5.1	21.3	1				197
Oxygen (-OH, -OR) ortho (except to -COOX)	0.5	2.1	+	0.0	0.0	5	1.5	6.3	+	
-OR ortho to -OR	3	12.6	2				2.3	9.6	2	198
-COOX ortho to alkyl (except t-bu), aryl, or O	3	12.6	+				1.0	4.2	+	
-COOX ortho to t-butyl	7	29.3	1				5.1	21.3	1	199
-COOX ortho to -COOX	6	25.1	3	6.5	27.2	8	6.1	25.5	+	200

Ring strain corrections (C-H-O)	Gas RSC			Liquid RSC			Solid RSC			Notes
	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	
Oxirane	27	113.0	2	24.0	100.4	9				201
Cyclopropanone	46.1	192.9	1							202
Cyclopropenone	101.7	425.5	1				94.6	395.8	1	203
Oxetane	25	104.6	2	22.3	93.3	1				204
1,2-Dioxetane	21.2	88.7	1							205
Cyclobutanone	27.9	116.7	1	25.1	105.0	2				206
Cyclobutanedione	32.1	134.3	1				24.7	103.3	1	207
Cyclobutenone							27.4	114.6	1	208
Cyclobutenedione	16.2	67.8	1	15.4	64.4	1	1.8	7.5	1	209
2-Oxetanone	24	100.4	1	18.1	75.7	1				210
Diketene	21.8	91.2	1	25.5	106.7	1				211
Tetrahydrofuran	5.9	24.7	2	4.0	16.7	2	5.3	22.2	4	212
Tetrahydrofuran-2-one	8.5	35.6	1	2.2	9.2	1				213
2,5-Dihydrofuran	4.2	17.6	1							214
2,3-Dihydrofuran	7.8	32.6	1							215
1,3-Dioxolane	5.3	22.2	4	5.7	23.8	5				216
1,3-Benzodioxole	14.3	59.8	1	17.6	73.6	1				217
Furan	-5.8	-24.3	9	-6.0	-25.1	7	-6.0	-25.1	4	
Cyclopentanone	6.2	25.9	1	1.9	7.9	2				218
Ascorbic acid							8.5	35.6	1	219
Succinic anhydride	0.8	3.3	4	1.0	4.2	4	7.4	31.0	+	
3,5-Cycloheptadien-1-one	6.9	28.9	1							220
2,5-Furandione	3.3	13.8	2	-2.4	-10.0	1	1.7	7.1	2	221
Phthalic anhydride	5.7	23.8	1				7.6	31.8	1	222
Benzofuran	-6.4	-26.8	1							223
Dibenzofuran	3.9	16.3	1				-1.0	-4.2	1	224
1,3-Dioxolane-2-one	10.8	45.2	2	-0.4	-1.7	2	-8.0	-33.5	1	225
1,3-Dioxol-2-one	7	29.3	2	-2.9	-12.1	2				226
1,2,4-Trioxolane							0.4	1.7	1	227
Tetrahydro-2H-pyran	1.1	4.6	3	-0.3	-1.3	3	-0.5	-2.1	+	228
1,3-Dioxane	1	4.2	8	1.0	4.2	+				
1,4-Dioxane	3.5	14.6	2	2.0	8.4	1				229
1,3,5-Trioxane	3.1	13.0	2	-2.3	-9.6	1	5.6	23.4	1	230
Dihydro-benzo-1,4-dioxin	-0.7	-2.9	1	2.3	9.6	1				231
Dihydro-2H-pyran	1.3	5.4	3			1				232
Epoxynaphthalene							13.0	54.4	1	233
Benzopyran	-14.8	-61.9	1							234
Benzo-1,4-dioxin	-25.5	-106.7	2							235
Dibenzopyran	1.4	5.9	1				-6.0	-25.1	1	236
Cyclohexanone	2.7	11.3	2	-0.7	-2.9	1				237
1-Tetralone							4.1	17.2	1	238
9,10-Anthracenedione	-9.8	-41.0	4				-12.6	-52.7	4	
9,10-Phenanthrenedione	-24.4	-102.1	1				-24.2	-101.3	1	239
1,2-Benzanthracene-9,10-dione	-20.5	-85.8	1				-40.4	-169.0	1	240
Tetrahydropyran-2-one	10.9	45.6	1	4.5	18.8	1				241

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 7

Ring strain corrections (C-H-O)	Gas RSC			Liquid RSC			Solid RSC			Notes
	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	
Xanthone	-5.9	-24.7	1				-12.3	-51.5	1	242
Glutaric anhydride	4.8	20.1	1				10.4	43.5	1	243
1,4-Cyclohexadien-dione	9.8	41.0	1				9.6	40.2	1	244
1,4-Naphthalenedione	18.5	77.4	2				-7.1	-29.7	2	245
Dibenzocyclohexanone	-4.3	-18.0	1							246
1,3-Dioxepane	7.5	31.4	1	4.6	19.2	1				247
Cyclohepten-7-one	-4	-16.7	1				0.8	3.3	1	248
Cycloheptatrien-one	0.6	2.5	2	3.4	14.2	1	-2.3	-9.6	2	249
Cycloheptanone	2.9	12.1	1	-0.5	-2.1	1				250
Dodecahydro-6,19-methanobenzo... cyclooctadecen-21-one	-1.9	-7.9	1				16.9	70.7	1	251
1,5-Benzodioxepin	8.7	36.4	1	11.6	48.5	1				252
1,3-Dioxocane	14.8	61.9	1	12.8	53.6	1				253
1,3,6-Trioxacyclooctane	8.7	36.4	1	5.0	20.9	1				254
Tetraoxane	13	54.4	1				6.7	28.0	1	255
Cyclooctanone	2	8.4	2	-0.8	-3.3	1	22.3	93.3	2	256
Cyclononanone	5.3	22.2	1	3.3	13.8	1	26.6	111.3	1	257
11-Oxabicyclo[4.4.1]undeca-pentaene	7.5	31.4	1	5.8	24.3	1	2.0	8.4	1	258
Cyclodecanone	4.2	17.6	1	2.1	8.8	1				259
Pentaoxecane	12.6	52.7	1				10.0	41.8	1	260
Cycloundecanone	5.1	21.3	1	2.7	11.3	1				261
1,4,7,10-Tetraoxacyclododecane (12-Crown-4)	9.2	38.5	1	6.7	28.0	1				262
Cyclododecanone	3.7	15.5	1	2.1	8.8	1	24.5	102.5	1	263
1,4,7,10,13-Pentaoxacyclopentadecane	8.9	37.2	1	6.4	26.8	1				264
Cyclopentadecanone	3	12.6	1				31.1	130.1	1	265
Benzo-15-crown-5-ether	-10.2	-42.7	1							266
Cycloheptadecen-2-one	-8.7	-36.4	1				4.9	20.5	1	266
Cycloheptadecanone	2.1	8.8	1				34.5	144.3	1	267
Anthracene peroxide							22.7	95.0	1	268
7-Oxabicyclo-[2.2.1]-heptane	14.2	59.4	1	10.0	41.8	1				269
Bicyclo-[2.2.1]-heptan-2-one	15	62.8	2				30.0	125.5	2	270
Bicyclo-[2.2.1]-heptan-7-one	23	96.2	1				38.1	159.4	1	271
Bicyclo-[3.3.0]-octan-2-one	8	33.5	2	4.0	16.7	2				271
Bicyclo-[2.2.2]-octanone	13.6	56.9	1							272
3-Oxabicyclo-[3.2.2]-nonane	11.6	48.5	1				5.2	21.8	1	273
Pyrano-[2,3-b]pyran-2,7-dione							124.0	518.8	2	274
Pyrano-[4,3-b]pyran-2,5-dione							105.0	439.3	2	275
Pyrano-[3,2-b]pyran-2,8-dione							95.0	397.5	1	276
2,4,8,10-Tetraoxospiro-[5.5]undecane	10.2	42.7	1				-9.4	-39.3	1	277
Epoxyconduritol (anhydro-alloinositol)							14.4	60.2	1	278
Butanolactone	9	37.7	1	2.4	10.0	1				279
4-Pentanolactone	8.5	35.6	1	2.2	9.2	1				280
5-Pentanolactone	10.9	45.6	1	4.5	18.8	1				281
Adamantan-2-one	9.8	41.0	1				22.1	92.5	1	282
Diamantanone	18	75.3	1				31.2	130.5	1	283
Inden-2-one	7.1	29.7	4	1.9	7.9	3	25.0	104.6	1	283
Benzopentaphene-5,8-dione	-63.6	-266.1	1				-54.9	-229.7	1	284
1,4,4a,8a-Tetrahydro-1,4-methano... naphthalene-5,8-dione							21.6	90.4	1	285
4b,10a-Dihydro-benzo[b]benzo[3,4]... cyclobuta[1,2-e][1,4]dioxin	12.5	52.3	1							286
8,9,10,11-Tetrahydro-6,12-methano-7H-... benzo-cycloundecene-14-one	38.6	161.5	1				46.6	195.0	1	287
Santonin							9.7	40.6	2	
3a,4,7,7a-Tetrahydro-4,7-methano-... isobenzofuran-1,3-dione	21.7	90.8	1				24.5	102.5	1	288
5,12,6,11-Bisepidioxy-5,6,11,12-tetrahydro-naphthacene							22.7	95.0	1	289
5,12-Dihydro-5,12-epidioxy-naphthacene							38.0	159.0	1	290

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 8

Ring strain corrections (C-H-O)	Gas RSC			Liquid RSC			Solid RSC			Notes
	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	kcal/mol	kJ/mol	#	
4b,9,10-triphenyl-indeno-[1,2,3-fg]-naphthacene-9-yl							58.2	243.5	1	291
Indeno[2,1-b]pyran	-2.2	-9.2	2				-4.4	-18.4	2	292
Dihydro-1-benzopyran	1.8	7.5	1				9.6	40.2	1	293
Dihydro-2-benzopyran	9.6	40.2	1				-1.0	-4.2	1	294
Endo-ethylene cyclohexanone	5.2	21.8	1	4.6	19.2	1				295
Anthradiquinone	32	133.9	1				35.2	147.3	1	296
Epoxycyclopentane	30	125.5	1	26.1	109.2	1				297
Epoxycyclohexane	28.2	118.0	1	23.8	99.6	1				298
Epoxycycloheptane	26.8	112.1	1	22.4	93.7	1				299
Epoxycyclooctane	28.7	120.1	1	24.9	104.2	1				300

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 1 n

Notes

1 s: C15H18 (1). It also occurs in 2,3,4-Trimethyl-indeno[2,1-b]pyran, but the latter is not used in evaluating the GAV.
2 l: GAV occurs only in 5-isopropylidenecyclopentadiene [C8H10 (6)], which is also only source for the Ful RSC.
3 g, l, s: Assigned the same values as C-(C)(H)3.
4 s: GAV based on C10H16 (15) (Camphene) only.
5 s: GAV based only on 1,3,5-cycloheptatriene, which is also only source for cycloheptatriene RSC. The GAV is as large as it can be without the RSC becoming negative, but still seems too small compared to the other phase GAVs.
6 g: GAV based on (Z)-5-ethylidene-bicyclo[2.2.1]-2-heptene, triquinacine, and dihydrotriquinacine; l: GAV found only in the first of these. All three are questionable experimental values.
7 g, l: GAVs based on norbornadiene (C7H8 (4)) only.
8 g: Allene, 1,2-butadiene, 3-methyl-1,2-butadiene, 1,2- and 2,3-pentadiene; l: 1,2-butadiene, 2,3-pentadiene, and 3-methyl-1,2-butadiene.
9 g: 2,7-Dimethyl-oct-1,7-dien-3,5-diyne, 2,4-hexadiyne, and C12H18 (2); GAV based only on latter; l: C18H18 (2); s: C12H18 (7) and C16H10 (
10 g, l, s: Assigned the same values as C-(C)(H)3.
11 s: GAV based only on 1,8-cyclotetradecadiyne, which is also only source for cyclotetradecadiyne RSC.
12 g: 2-Methyl-1-buten-3-yne, C6H10 (10), 2,7-dimethyl-oct-1,7-dien-3,5-diyne, and C12H18 (4); l: C6H10 (10) and C12H18 (4); s: C12H18 (7).
13 l: C7H8 (5).
14 g: 2-Methyl-1-buten-3-yne and 2,7-dimethyl-oct-1,7-dien-3,5-diyne.
15 g, l, s: Assigned the same values as C-(C)(H)3.
16 g: C26H22 (2); l: C14H14 (3), C16H18 (1), and C16H18 (3).
17 s: Group found only in 2,2-bis(4-hydroxyphenyl)-propane; l: based on 2,2-diphenylbutane, which is cited by SWS and is of questionable reliability.
18 g, s: GAV based solely on triphenylmethane; difference between phases seems too large. GAV also occurs in C20H14 (1), which was not used in evaluation.
19 g, s: Occurs in 1,1,1-triphenylethane, 1,1,1,2-tetraphenylethane, pentaphenylethane, and hexaphenylethane. Two of these values (in solid phase) seem inconsistent with the others.
20 g, s: Occurs only in tetraphenylmethane; difference between phases seems large, but it is not apparent which, if either, is wrong.
21 g: C8H6 (1), 1-phenyl-1-propyne, 1-phenyl-1-butyne, C14H10 (1); l: C8H6 (1); s: C14H10 (1), C16H10 (1), C16H14 (1, 2).
22 l: C9H10(2) and C12H14(2), GAV is based on former only; s: C25H20(2). Benson (Thermochemical Kinetics, 1976, p. 272, reports a value of 36.15 kJ/mol for gas phase GAV.
23 g: C14H12 (2) and C18H14 (2); l: C14H12 (2).
24 g: 2,3,4-Trimethyl-indeno[2,1-b]pyran and 6-phenylindeno[2-1,b]pyran; s: these two and C25H20 (2), C28H22 (2). The first two of these also are the only compounds with the indeno[2-1,b]pyran RSC, so only the sum of the GAV and RSC can be determined. The gas phase GAV is set equal to the solid phase value.
25 l: C8H6 (1).
26 g: C9H8 (1); l: C9H8 (1) and C9H10 (4).
27 l: Group found only in 3-phenyl-1-butene.
28 g, s: Group found only in pyrene and perylene, and there is 20-25 kJ/mol discrepancy between the two.
29 g: C3H4 (3) and C4H6 (7).
30 g: C4H6 (6); l: Dimethylmethylenecyclopropane, which is of questionable reliability.
31 g, l: C5H8 (11).
32 g: C4H6 (5) and 3,4-dimethylenecyclo-1-butene; RSC based on former; s: C22H28O (2).
33 s: Fused five-membered rings in triquinacines have a separate RSC (Trq).
34 s: C10H12 (2) and C10H14 (8). There are 2 additional cyclopentene compounds (both C8H14s) in liquid phase not used in evaluating this RSC.
35 g, l: C5H6 (3).
36 l: C7H10 (2), C10H16 (9), and 1-ethyl-4-methyl-1,3-cyclohexadiene.
37 g: 1,4-Cyclohexadiene; 3-methylene-1,4-cyclohexadiene, and 3,6-bis(methylene)-1,4-cyclohexadiene. l: 1,4-Cyclohexadiene.
38 l: 1-Methyl-3-methylene-1-cyclohexene. The value for this compound is of questionable reliability.
39 g: GAV depends only on cycloheptane; ethylcycloheptane was not used for GAV evaluation.
40 g: C7H12 (6).
41 g, l: C7H10 (3).
42 l: 1,4-Cycloheptadiene.
43 g, l: Cycloheptatriene; s: RSC depends only on 1,3,6-triphenyl-1,3,5-cycloheptatriene, which is also only source for C-(Cd)2(H)2.
44 g, l: C8H16 (17).
45 g, l: C8H14 (5).
46 l: (E)-Cyclooctene.
47 g, l: C8H12 (9)
48 g, l: C8H8 (1).
49 g, l: C9H18 (3).
50 l: (Z)-Cyclononene.
51 l: (E)-Cyclononene.
52 l: (Z,Z,Z)-1,4,7-Cyclononatriene.

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 2 n

53 g: Cyclodecane.
54 l: (Z)-Cyclodecene.
55 l: (E)-Cyclodecene.
56 g, l: C11H22 (2).
57 g: C12H24 (1).
58 g, l: C12H18 (5).
59 g, s: C12H18 (6).
60 g, l: C13H26 (2).
61 g, s: C14H28 (1). Gas phase value has been adjusted based on other cycloalkanes; see N. Cohen and S. W. Benson, Chem. Rev. 93, 2419 (1993).
62 s: RSC depends only on 1,8-cyclotetradecadiyne, which is also only source for C-(C)(Ct)(H)2 GAV.
63 g, s: C15H30 (2).
64 g, s: C16H32 (3).
65 s: C16H16 (10).
66 g, s: C17H34 (1).
67 s: C18H18 (1).
68 g, l: C6H10 (9) and C7H12 (9).
69 l: Bicyclo[2.2.1]hex-2-ene.
70 g, l: C10H16 (3 and 4).
71 g: 7-Phenyl-bicyclo[3.2.0]hept-2-en-6-ol
72 g: Norbornene and C10H12 (3); s: Norbornene and C10H12 (2).
73 g, l: C8H14 (7).
74 g, l: C8H14 (6).
75 s: C8H12 (2).
76 g, l: (Z)-Bicyclo[3.3.0]octane (Octahydropentalene).
77 g, l: (E)-Bicyclo[3.3.0]octane.
78 g, l: C9H16 (4 and 6).
79 g, s: C9H16 (11).
80 g, s: Bicyclo[3.3.1]-2-nonene
81 g, s: Bicyclo[3.2.2]-6-nonene
82 g, s: Bicyclo[4.2.1]-3-nonene
83 g, s: C10H18 (6).
84 Perhydroazulene (Bicyclo[5.3.0]decane)
85 g: C10H12(3); s: C10H12 (2).
86 l: Tetracyclo[5.2.1.0^2,6.0^3,5]-8-decene.
87 g: Bicyclo-[3.3.3]-undecane
88 g, l: Bicyclo-[4.4.1]-undecane
89 g, l: C9H8 (1).
90 g, l: C10H16 (11); s: C10H14 (8) and C10H16 (11).
91 g: 1,2-Cyclobutylbenzene.
92 g: Benzocyclopropene and 2,3-cyclopropylnaphthalene
93 g, l: 1,2-Dihydronaphthalene.
94 l: 1,4-Dihydronaphthalene.
95 g, s: C12H8 (1).
96 g, l: Spiropentane.
97 g: Fulvene, C8H10 (6), and 6,6-diphenylfulvene; discrepancy is over 25 kJ/mol. l: C8H10 (6); s: 6,6-Diphenylfulvene.
98 g: Azulene; s: Azulene and C15H18 (1).
99 l: Diamantane; the RSC does not appear consistent with the g and s values.
100 g, s: Fluoranthene.
101 g, s: Acenaphthene. Acenaphthylene uses the same RSC here, though it might require its own RSC.
102 g: Triquinacine, dihydrotriquinacine, and tetrahydrotriquinacine. The latter two should probably have their own RSCs.
103 g, s: Perhydroquinacine.
104 s: Dodecahydrotriphenylene.
105 g, s: 9,10-Dihydro-9,10[1',2']-benzenoanthracene.
106 g, s: 9,10-Dihydroanthracene and 5,12-dihydronaphthacene.
107 l: 9,10-Dihydrophenanthrene.
108 g, l, s: Octahydroanthracene.
109 g, l: 1,2,3,4-Tetrahydronaphthalene; s: 1,2,3,4- and 5,6,7,8-tetrahydro-1-naphthol.
110 s: C14H24 (1) and C14H28 (2); NNI value based primarily on the latter, though there is some uncertainty.
111 l: C10H20 (2).
112 g: C6H12 (17); l: C6H12 (17) and 2,3-dimethyl-2-pentene; s: 6,6-diphenylfulvene (C18H14 (2)). The latter is a poor model for this cis interaction because the 1 and 4 carbons of the ring are farther from the other end of the external =C than would be the case if the compound were acyclic.
113 g, l: NNI value based on C5H6 (1) and C10H16 (1).
114 g: C18H30 (1); s: C18H30 (1) and C22H38 (1).

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 3 n

115 Note: for a single CH3 on the 4 or 5 position, use 1/2 of correction.
116 l: C12H12 (1) and C14H16 (1).
117 g,l,s: group occurs only in H2O.
118 g: Estimated by comparison with O-(C)(H). This GAV and that for Ct-(O) together sum to -29 kJ/mol based on data for 2-propyn-1-ol as compiled by M. S. Kharasch (J. Res. N.B.S. 2, 359 [1929]), and of questionable reliability.
119 s: 1,3-Diphenyl-3-ethoxy-2-propen-1-one.
120 l: Diphenyl ether.
121 l: Phenyl vinyl ether.
122 g: C4H4O2 (2) and C4H6O2 (2); l: same two and C5H8O2 (6). GAV's are averages. Discrepancy in gas phase is 15.9 kJ/mol; 28.9 kJ/mol in liquid.
123 g: ethyl, 1-methyl-1-phenylethyl, and t-butyl hydroperoxide, and H2O2. Because H2O2 may be abnormal, and in view of large discrepancies among the data in all 3 phases, the GAV is based mainly on t-BuOOH.
124 s: The five compounds with this group are so discordant that they are not useful for GAV evaluation. The value chosen here is based solely on dioxybismethanol, the only one of the five that looks like it has a chance of being correct.
125 g: estimated by comparison with similar groups; s: 1,2,3,4-Tetrahydro-5-hydroperoxynaphthalene.
126 g: C16H16O3 (1), C14H10O4 (1), C14H10O5 (1), C14H16O5 (1). There is discrepancy of 63 kJ/mol among these 4 compounds, so there is considerable uncertainty in GAV.
127 g: P. S. Nangia and S. W. Benson, J. Phys. Chem. 83, 1138 (1979); updated by S. W. Benson and N. Cohen, in press. l: estimated.
128 g, l, s: Assigned the same values as C-(C)(H)3.
129 g: C5H12O2 (1), C7H14O2 (9), and C7H16O2 (1); discrepancy is only 13 kJ/mol.
130 g, l: 1,1,1-trimethoxymethane.
131 g, l: C4H10O3 (2) and C7H16O3 (1); discrepancy is small.
132 g, l: Tetramethoxymethane (Tetramethyl orthocarbonate); tetraethoxymethane.
133 l: Based on Allyl alcohol; other two compounds are from 63PAS/GAR (PNK's reference), an unrefereed and unreliable source.
134 g, s: 2-(Diacetoxymethyl)furan.
135 g: 2-Methyl-3-buten-2-ol and 2,2-dimethyl-2H-1-benzopyran. The latter has the only benzopyran RSC, so GAV is based on former; RSC on latter.
136 s: C15H18O3 (1), C6H10O4 (9), C6H8O6 (1). The last has the only ascorbic acid RSC, so other 2 determine GAV; discrepancy is 23 kJ/mol; the 2nd one, which has 2 of the groups, is used. l: C7H10O2 (6), C6HC6H10O (2), C7H12O (4); the latter two are from an unreliable and unrefereed source (63PAS/GAR), so GAV is based on the first one.
137 s: C8H14O2 (12) and C12H22O2 (1); discrepancy is 21.8 kJ/mol, use average.
138 g: 1-tert-Butyl-4-(2-propynyloxy)-benzene. l: Based on 2-octyn-1-ol, 2-nonyn-1-ol, and 1-phenyl-1-propyn-3-ol; the spread is 41 kJ/mol; data compiled by Kharasch.
139 g, l: 3-Pentynoic acid ethyl ester; s: 3-butynoic acid.
140 s: Acetylenedicarboxylic acid dihydrate.
141 g: (Methoxymethyl)-benzene and C27H22O3 (1); 2 groups in latter, so use it to determine GAV. s: C8H10O2 (2) and C27H22O3 (1); no disagreement.
142 s: 3,5-Diphenyl-1,2,4-trioxolane. This is the only source for this GAV, as well as for the 1,2,4-trioxolane RSC.
143 s: 9,10-Epidioxyanthracene.
144 l: 1-Phenyl-2-propanone.
145 s: 2-Hydroxy-1,2-diphenylethanone.
146 g: Cyclopropyl phenylmethanol and 4b,10a-dihydro-benzo[b]benzo[3,4]-cyclobuta[1,2-e]dioxin.
147 g, s: C9H12O2 (1) and C16H26O3 (1). Discrepancies are 47.7 and 18.8 kJ/mol in two phases, resp.; use averages; l: 1-Methyl-1-phenylethylhydroperoxide.
148 s: Benzhydrol (diphenyl methanol).
149 s: C19H16O (1), C22H22O (1), C38H30O2 (1), and C42H28O2 (3). The discrepancy among these is large, and the GAV is based mainly on the first one.
150 g, s: 3',5'-Diisopropyl-4,4-dimethyl-3-phenyl-1,2-benzocyclobutene-3-ol.
151 g: alpha-Ethenyl-benzenemethanol.
152 s: 5,12,Dihydro-5,6,11,12-tetraphenyl-5,12-epidioxy-naphthacene.
153 s: l-Sorbose.
154 s: Benzoyl acetone, C15H12O2 (1), C4H4O2 (3), and C3H4O4 (1); the last has large error, so GAV based on first three.
155 g, l, s: Assigned the same values as C-(C)(H)3.
156 g, s: 2,2,4,4-Tetramethyl-1,3-cyclobutanedione.
157 g: 1-(3,4-Dihydro-6-methyl-2H-pyran-2-yl)-ethanone; s: C3H6O3 (2) and C6H12O6 (2); use average-- discrepancy is 19.2 kJ/mol.
158 s: Furoin: based on data compiled by M. S. Kharasch (J. Res. N.B.S. 2, 359 [1929]), and of questionable reliability.
159 s: Dimethyl tartrates.
160 s: Dihydroxymalonic acid; based on data compiled by M. S. Kharasch (J. Res. N.B.S. 2, 359 [1929]), and of questionable reliability.
161 s: C5H6O4 (2), C6H6O6 (1) and C6H6O6 (2); average of all three.
162 l: 1,1,3-Triphenyl-2-propyn-1-ol; based on data compiled by M. S. Kharasch (J. Res. N.B.S. 2, 359 [1929]), and of questionable reliability.
163 l: Acetylmalonic acid dimethyl ester; based on data compiled by M. S. Kharasch (J. Res. N.B.S. 2, 359 [1929]), and of questionable reliability.
164 s: Tartronic acid: based on data compiled by M. S. Kharasch (J. Res. N.B.S. 2, 359 [1929]), and of questionable reliability.
165 g, l: Methyl, propyl, and phenyl esters of formic acid. Propyl disagrees with others by 50 kJ/mol; GAV based on methyl.

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 4 n

166 g: C2H2O2 (1) and C3H4O2 (1); discrepancy is 8 kJ/mol; use weighted average; l: 1,2-Propanedione (Pyruvaldehyde).
167 g: C3H4O2 (1), C4H6O2 (1), C18H10O2 (2), and C3H4O3; use weighted average. s: 2-Oxopentanedioic acid.
168 l: C4H6O4 (3), C6H10O4 (7), and C14H10O4 (2).
169 s: C17H30O (1), C8H8O2 (13), C11H10O2 (1), and 3-phenylcyclobutenone.
170 s: 3-(2-Furyl)-2-propenal.
171 l: 2,4,6-Cycloheptatrien-1-one.
172 g: 2-Pentynoic acid ethyl ester; s: C5H6O2 (1) and C4H2O4 (1); use weighted average; discrepancy less than 4 kJ/mol.
173 g: C8H8O2 (3) and C7H6O (1); small discrepancy. s: C8H8O2 (1) and C8H8O3 (1); discrepancy is 15.9 kJ/mol; use average.
174 l: C13H10O (2), C15H14O (1), and C17H18O (1).
175 g, s: C14H8O2 (2) and C14H10O2 (1). The former has a unique ring, so the latter is used to determine GAVs.
176 g: C10H6O2 (1) and C10H6O4; small discrepancy, use average.
177 g, l: 3,4-Diethoxy-3-cyclobutene-1,2-dione; s: 3,4-Dihydroxy-3-cyclobutene-1,2-dione.
178 g: But-1-yn-3-one. l: 1-Phenyl-pent-1-yn-3-one; based on data compiled by Kharasch.
179 s: C9H10O5 (1) and C6H8O6 (1). Both compounds have unique groups, so this GAV is estimated by comparison with liquid phase GAV.
180 l: C6H6O (2), C10H8O (3), and C3H2O3 (1).
181 l: C5H4O2 (1), C6H6O3 (2), and C8H10O4 (1).
182 s: 1,3-Diphenyl-3-ethoxy-2-propen-1-one.
183 g, s: Diphenylcyclopropenone. This molecule also has the only C3d=O RSC.
184 g: 2-Methylene-3-butenoic acid ethyl ester and 3-furancarboxylic acid; l: the former. Discrepancy in gas phase is 29 kJ/mol.
185 g: 1,4,9,10-Anthradiquinone. s: Benzylidenemalonic acid: based on data compiled by Kharasch.
186 g: But-1-en-3-yn-2-ol.
187 g, l: Ketene.
188 g: Methyl ketene.
189 g: 2-Methyl-1-propen-1-one.
190 g: Phenyl ethenone (Phenyl ketene).
191 g: Diphenyl ethenone.
192 g, l, s: Assigned the same values as C-(C)(H)3.
193 g: Phenyl ethenone and diphenyl ethenone.
194 g: 2-Propyn-1-ol; see note 109.
195 g: But-1-yn-3-one and C7H10O2 (4); former has only CO-(C)(Ct) group, so it determines latter GAV; C7H10O2 (4) establishes this GAV; s: 3-Pentynoic acid.
196 g, l: Di-tert-butyl ether.
197 g, l: Di-tert-butyl ketone.
198 g, s: Dimethoxy benzoic acids.
199 g, s: 2-tert-butyl benzoic acid.
200 Note: 2 C(O)O groups in cis configuration on a five-membered ring seem to require about half of this ortho correction.
201 g: Oxirane and methyloxirane.
202 g: Oxiranone.
203 g, s: Diphenylcyclopropenone. This molecule also has the only Cd-(Cb)(CO) group.
204 g: Oxetane and 3,3-Dimethyloxetane; l: 3,3-Dimethyloxetane.
205 g: 3,3,4,4-Tetramethyl-1,2-dioxetane.
206 g, l: Cyclobutanone. Phenylcyclobutanone (l) was not used to evaluate RSC.
207 g, l: 3,4-Diethoxy-3-cyclobutenedione; s: 3,4-Dihydroxy-3-cyclobutenedione.
208 s: 3-Phenylcyclobutenone.
209 g, s: Cyclobutane-1,3-dione.
210 g, l: 2-Oxetanone (beta-Propiolactone).
211 g, l: Diketene.
212 g, l: Tetrahydrofuran and C5H10O2 (9).
213 g, l: Tetrahydrofuran-2-one.
214 g: 2,5-Dihydrofuran.
215 g: 2,3-Dihydrofuran.
216 g: 1,3-Dioxolane, 2-Methyl-1,3-dioxolane and the 2,4-dimethyl-1,3-dioxolanes; l: all of these and 2,2-dimethyl-1,3-dioxolane.
217 g, l: Methylenedioxybenzene (1,3-Benzodioxole).
218 g: Cyclopentanone; l: cyclopentanone and 2-methylcyclopentanone.
219 s: l-Ascorbic acid.
220 g: 3,5-Cycloheptadien-1-one.
221 g: 2,5-Furandione and 3-methyl-2,5-furandione; l: 3-methyl-2,5-furandione; s: 2,5-furandione (3,4-dimethyl-2,5-furandione is inconsistent by 42 kJ/mol).
222 g, s: Phthalic anhydride
223 g: Benzofuran.
224 g, s: Dibenzofuran.
225 g, l: C3H4O3 (1) and C3H8O3 (1); s: C3H4O3 (1).
226 s: 1,3-Dioxolane-2-one.
227 s: 3,5-Diphenyl-1,2,4-trioxolane. This is the only source for this RSC, as well as for the C-(Cb)(H)(O)2 group.
228 g, l: Tetrahydro-2H-, tetrahydro-2-methoxy-, and 2-(2-methoxy)-tetrahydro-2H-pyran.

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 5 n

229 g, l: 1,4-Dioxane.
230 l: Trimethyl-1,3,5-dioxane; s: 1,3,5-trioxane; g: both (there is a discrepancy of more than 50 kJ/mol between the two; K. Pihlaja and M.-L. Tuomi (Suomen Kemistilehti, B43, 224 (1970)) attribute this to "excess stabilization" in the methylated compound.
231 g, l: C8H8O2 (11).
232 g, Dihydro-2H-pyran, 6-methoxy-dihydro-2H-pyran; l: dihydro-2H-pyran; gas value for 2-ethoxy-3,4-dihydro-6-methoxy-2H-pyran is not consistent.
233 s: 1,4-Dihydro-1,4-epoxynaphthalene.
234 g: 2,2-Dimethyl-2H-1-benzopyran.
235 g: 2-Phenyl-1,4-benzodioxin and 2,3-diphenyl-1,4-benzodioxin.
236 g, s: Dibenzopyran.
237 g: C6H10O (4); l: C6H10O (4) and C7H12O (1).
238 s: 1-Tetralone.
239 g, s: 9,10-Phenanthrenedione.
240 g, s: 1,2-Benzanthracene-9,10-dione.
241 g, l: Tetrahydro-2H-pyran-2-one.
242 g, s: Xanthone (Xanthen-9-one).
243 g, s: Glutaric anhydride.
244 g, s: 2,5-Cyclohexadien-1,4-dione.
245 g, s: 1,4-Naphthalenedione and 5,8-Dihydroxy-1,4-naphthoquinone.
246 g: Dibenzocyclohexanone.
247 g, l: 1,3-Dioxepane.
248 g, s: C13H12O (2).
249 g: 2,4,6-Cycloheptatrien-1-one, 2-Hydroxy-2,4,6-cycloheptatriene-1-one (23.4 kJ/mol discrepancy); l: 2,4,6-Cycloheptatrien-1-one.
250 g, l: Cycloheptanone.
251 g, s: Dodecahydro-6,19-methanobenzo-cyclooctadecen-21-one.
252 g, l: 3,4-Dihydro-2H-1,5-benzodioxepin.
253 g, l: 1,3-Dioxocane.
254 g, l: 1,3,6-Trioxacyclooctane.
255 g, s: 1,3,5,7-Tetraoxane.
256 l: Cyclooctanone.
257 g, l: Cyclononanone.
258 g, l, s: 11-Oxabicyclo[4.4.1]undeca-pentaene.
259 g, l: Cyclodecanone.
260 g, s: Pentaoxecane.
261 g, l: Cycloundecanone.
262 g, l: 1,4,7,10-Tetraoxocyclododecane.
263 g, l, s: Cyclododecanone.
264 g, l: 1,4,7,10,13-Pentaoxacyclopentadecane.
265 g, s: Cyclopentadecanone.
266 g: Benzo-15-crown-5-ether
267 g, s: Cycloheptadecanone.
268 s: 9,10-Epidioxyanthracene.
269 g, l: 7-Oxabicyclo[2.2.1]heptane.
270 g, s: C7H10O (1) and C10H16O (1).
271 g, s: C7H10O (2).
272 g: Bicyclo-[2.2.2]-octanone.
273 g, s: 3-Oxabicyclo-[3.2.2]-nonane.
274 s: 4-Methyl-2H,7H-pyrano-[2,3-b]pyran-2,7-dione and 4,5-dimethyl-2H,7H-pyrano-[2,3-b]pyran-2,7-dione; GAV is based on the former (large discrepancy between the two).
275 s: 7-Methyl-2H,5H-pyrano-[4,3-b]pyran-2,5-dione and 4,7-dimethyl-2H,5H-pyrano-[4,3-b]pyran-2,5-dione.
276 s: 4,6-Dimethylpyrano-[3,2-b]pyran-2,8-dione.
277 g, s: 2,4,8,10-Tetraoxospiro-[5.5]undecane.
278 s: 1,2-Anhydro-3,4,5,6-alloinositol.
279 g, l: 4-Butanolactone.
280 g, l: 4-Pentalactone.
281 g, l: 5-Pentalactone.
282 g, s: Adamantan-2-one.
283 g, s: Diamantanone.
284 g, s: Benzo[rst]pentaphene-5,8-dione.
285 s: 1,4,4a,8a-Tetrahydro-1,4-methanonaphthalene-5,8-dione.
286 g: 4b,10a,Dihydro-benzo[b]benzo-[3,4]cyclobuta[1,2-e][1,4]dioxin.
287 g, s: 8,9,10,11-Tetrahydro-6,12-methano-7H-benzo-cycloundecene-14-one.
288 g, s: 3a,7,7,7a-Tetrahydro-4,7-isobenzofuran-1,3-dione.
289 s: 5,12,6,11-Bisepidioxy-5,6,11,12-tetrahydro-5,6,11,12-tetraphenyl-naphthacene.

Table 1. Group additivity values for enthalpy of formation (298 K), C-H-O groups, 6 n

290 s: 5,12-Dihydro-5,6,11,12-tetraphenyl-5,12-epidioxy-naphthacene.
291 s: 4b,9-Dihydro-9-hydroperoxy-4b,9,10-triphenyl-indeno-[1,2,3-fg]naphthacene-9-yl.
292 g, s: 2,3,4-Trimethyl-indeno[2,1-b]pyran and 6-phenylindeno[2,1-b]pyran. The discrepancy between the two is large; the latter is used for the RSC.
293 g, s: 3,4-Dihydro-2H-1-benzopyran.
294 g, s: 3,4-Dihydro-1H-2-benzopyran. The discrepancy between gas and solid phases--and with the preceding RSCs--is puzzling.
295 g, l: 2,5-Endo-ethylene cyclohexanone.
296 g, s: 1,4,9,10-Anthradiquinone.
297 g, l: (Z)-1,2-Epoxycyclopentane.
298 g, l: (Z)-1,2-Epoxycyclohexane.
299 g, l: (Z)-1,2-Epoxycycloheptane.
300 g, l: (Z)-1,2-Epoxycyclooctane.

Table 2. Comparison of group additivity values, Enthalpy of formation (298 K), 1

Group	Group Additivity Value						Group	Group Additivity Value					
	Gas		Liquid		Solid			Gas		Liquid		Solid	
	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol
C-(C)(H)3	-10.0	-41.8	-11.6	-48.5	-10.1	-42.3	C-(C)(Cd)(Ct)2						
C-(Cd)(H)3	-10.0	-41.8	-11.6	-48.5	-10.1	-42.3	C-(C)(Cb)3	4.3	18.0			30.0	125.5
C-(Cb)(H)3	-10.0	-41.8	-11.6	-48.5	-10.1	-42.3	C-(C)(Cd)3						
C-(Ct)(H)3	-10.0	-41.8	-11.6	-48.5	-10.1	-42.3	C-(C)(Ct)3						
							C-(Cb)4	7.3	30.5			17.5	73.2
C-(C)2(H)2	-5.0	-20.9	-6.1	-25.5	-7.0	-29.3	C-(Cd)4						
C-(C)(Cd)(H)2	-4.8	-20.1	-6.1	-25.5	-5.0	-20.9	C-(Ct)4						
C-(C)(Ct)(H)2	-4.7	-19.7	-5.3	-22.2	-7.1	-29.7	C-(Cb)2(Cd)2						
C-(C)(Cb)(H)2	-4.6	-19.2	-6.2	-25.9	-6.5	-27.2	C-(Cb)2(Ct)2						
C-(Cb)2(H)2	-6.3	-26.4	-5.2	-21.8	-6.0	-25.1	C-(Cd)2(Ct)2						
C-(Cd)2(H)2	-4.3	-18.0	-5.8	-24.3	-13.3	-55.6	C-(Cb)3(Cd)						
C-(Ct)2(H)2							C-(Cb)3(Ct)						
C-(Cb)(Cd)(H)2	-2.5	-10.5	-4.7	-19.7			C-(Cd)3(Ct)						
C-(Cb)(Ct)(H)2							C-(Cb)(Cd)3						
C-(Cd)(Ct)(H)2							C-(Cb)(Ct)3						
							C-(Cd)(Ct)3						
C-(C)3(H)	-2.4	-10.0	-2.2	-9.2	-4.0	-16.7	C-(Cb)(Cd)2(Ct)						
C-(C)2(Cd)(H)	-1.7	-7.1	-2.4	-10.0	-3.0	-12.6	C-(Cb)(Cd)(Ct)2						
C-(C)(Cd)2(H)	2.7	11.3	1.8	7.5			C-(Cb)2(Cd)(Ct)						
C-(Cd)3(H)													
C-(C)2(Ct)(H)	-1.8	-7.5	-2.0	-8.4									
C-(C)(Ct)2(H)							Cd-(H)2	6.3	26.4	4.9	20.5	6.0	25.1
C-(Ct)3(H)													
C-(C)2(Cb)(H)	-1.0	-4.2	-1.0	-4.2	-1.0	-4.2	Cd-(C)(H)	8.6	36.0	7.7	32.2	6.1	25.5
C-(C)(Cb)2(H)	-1.1	-4.6	-6.5	-27.2	5.6	23.4	Cd-(Cd)(H)	6.8	28.5	5.3	22.2	5.2	21.8
C-(Cb)3(H)	-1.0	-4.2			9.8	41.0	Cd-(Ct)(H)	6.7	28.0	4.7	19.7		
C-(C)(Cb)(Cd)(H)			-2.1	-8.8			Cd-(Cb)(H)	6.8	28.5	1.5	6.3	3.0	12.6
C-(Cb)2(Cd)(H)													
C-(Cb)(Cd)2(H)							Cd-(C)2	10.2	42.7	9.7	40.6		
C-(Cb)(Cd)(Ct)(H							Cd-(C)(Cd)	8.8	36.8	8.0	33.5	7.7	32.2
C-(Cb)2(Ct)(H)							Cd-(Cd)2	6.6	27.6	4.0	16.7	2.7	11.3
C-(Cb)(Ct)2(H)							Cd-(C)(Ct)	9.5	39.7				
C-(Cd2)(Ct)(H)							Cd-(C)(Cb)			5.7	23.8	5.0	20.9
C-(Cd)(Ct2)(H)							Cd-(Cb)2	8.0	33.5	7.2	30.1	9.6	40.2
							Cd-(Cb)(Cd)	13.0	54.4			13.2	55.2
C-(C)4	-0.1	-0.4	0.8	3.3	-1.5	-6.3							
C-(C)3(Cb)	2.9	12.1	3.4	14.2	0.4	1.7	Ct-(H)	27.2	113.8	26.0	108.8		
C-(C)3(Cd)	1.7	7.1	2.3	9.6	4.3	18.0							
C-(C)3(Ct)	1.3	5.4	1.9	7.9	0.5	2.1	Ct-(C)	27.3	114.2	25.5	106.7	23.9	100.0
C-(C)2(Cb)2			[10]	[42]	9.8	41.0	Ct-(Ct)	25.3	105.9	25.2	105.4	24.7	103.3
C-(C)2(Cd)2	6.8	28.5	5.2	21.8			Ct-(Cd)	27.9	116.7	28.0	117.2		
C-(C)2(Ct)2			3.5	14.6			Ct-(Cb)	24.6	102.9	26.5	110.9	23.5	98.3
C-(C)2(Cb)(Cd)													
C-(C)2(Cb)(Ct)							Cb-(H)	3.3	13.8	2.0	8.2	1.5	6.3
C-(C)2(Cd)(Ct)													
C-(C)(Cb)2(Cd)							Cb-(C)	5.5	23.0	4.8	20.1	2.9	12.1
C-(C)(Cb)2(Ct)							Cb-(Cd)	5.8	24.3	8.0	33.5	5.8	24.3
C-(C)(Cb)(Cd)2							Cb-(Ct)	5.7	23.8	5.5	23.0	5.5	23.0
C-(C)(Cb)(Ct)2							Cb-(Cb)	5.2	21.8	5.0	20.9	4.4	18.4
C-(C)(Cd)2(Ct)													

Table 2. Comparison of group additivity values, Enthalpy of formation (298 K), 2

Group	Group Additivity Value						Group	Group Additivity Value					
	Gas		Liquid		Solid			Gas		Liquid		Solid	
	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol
C-(H)3(O)	-10.0	-41.8	-11.6	-48.5	-10.1	-42.3	C-(C)3(O)	-6.6	-27.6	-5.6	-23.4	-5.6	-23.4
C-(H)2(O)2							C-(Cb)3(O)					18.0	75.3
C-(H)(O)3	-26.8	-112.1	-25.3	-105.9			C-(Cd)3(O)						
C-(O)4	-38.6	-161.5	-36.7	-153.6			C-(Ct)3(O)						
							C-(C)2(Cb)(O)	-4.2	-17.6	1.8	7.5	17.9	74.9
C-(C)(H)2(O)	-8.1	-33.9	-9.1	-38.1	-5.0	-20.9	C-(C)2(Cd)(O)	13.0	54.4				
C-(Cb)(H)2(O)	-12.4	-51.9			-3.0	-12.6	C-(C)2(Ct)(O)					1.5	6.3
C-(Cd)(H)2(O)	-6.9	-28.9	-8.0	-33.5			C-(Cb)2(Cd)(O)					-2.0	-8.4
C-(Ct)(H)2(O)	-8.6	-36.0	[-6]	[25]			C-(Cb)2(Ct)(O)			[2.5]	[10]		
C-(H)2(O)(CO)					-4.6	-19.2	C-(Cd)2(Ct)(O)						
C-(H)2(O)(CCO)							C-(C)(Cb)(Cd)(O)	-4.7	-19.7			7.2	30.1
							C-(C)(Cb)(Ct)(O)						
C-(C)2(H)(O)	-7.2	-30.1	-7.0	-29.3	-1.0	-4.2	C-(Cb)(Cd)(Ct)(O)						
C-(Cb)2(H)(O)					-1.0	-4.2							
C-(Cd)2(H)(O)							C-(C)(O)3	-25.5	-106.7	-24.7	-103.3		
C-(Ct)2(H)(O)							C-(Cb)(O)3						
C-(C)(Cb)(H)(O)	-4.4	-18.4			0.1	0.4	C-(Cd)(O)3						
C-(C)(Cd)(H)(O)			-29.2	-122.2	-5.0	-20.9	C-(Ct)(O)3					26.4	110.6
C-(C)(Ct)(H)(O)							C-(O)3(CO)						
C-(Cb)(H)(O)(CO					7.9	33.1	C-(O)3(CCO)						
C-(Cb)(Cd)(H)(O)	-4.8	-20.1											
C-(Cb)(Ct)(H)(O)							C-(C)2(H)(CO)	-1.7	-7.1	-1.4	-5.9	-9.0	-37.7
C-(Cd)(Ct)(H)(O)							C-(Cb)2(H)(CO)						
C-(C)(H)(O)(CO)	-4.5	-18.8			-6.9	-28.9	C-(Cd)2(H)(CO)						
C-(Cd)(H)(O)(CO					[10]	[40]	C-(Ct)2(H)(CO)						
C-(H)(O)(CO)2					[-9.5]	[-40]	C-(C)(H)(CO)2					-14.0	-58.6
C-(C)(H)(O)(CCO							C-(C)(Cb)(H)(CO)					1.0	4.2
							C-(C)(Cd)(H)(CO)						
C-(C)(H)(O)2	-15.8	-66.1	-16.0	-66.9	-20.0	-83.7	C-(C)(Ct)(H)(CO)						
C-(Cb)(H)(O)2					0.1	0.4	C-(Cb)(Cd)(H)(CO)						
C-(Cd)(H)(O)2	-0.3	-1.3			-7.0	-29.3	C-(Cb)(Ct)(H)(CO)						
C-(Ct)(H)(O)2							C-(Cd)(Ct)(H)(CO)						
C-(H)(O)2(CO)													
C-(H)(O)2(CCO)							C-(C)(H)2(CO)	-5.2	-21.8	-5.2	-21.8	-14.6	-61.1
							C-(Cb)(H)2(CO)	-5.4	-22.6	-3.1	-13.0	-3.0	-12.6
C-(C)2(O)2	-16.2	-67.8	-15.8	-66.1			C-(Cd)(H)2(CO)	-3.8	-15.9	-8.0	-33.5	-15.0	-62.8
C-(Cb)2(O)2					54.0	225.9	C-(Ct)(H)2(CO)	-5.0	-20.9	-4.9	-20.5	15.2	63.6
C-(Cd)2(O)2							C-(H)2(CO)2	-6.6	-27.6	-5.8	-24.3	-8.0	-33.5
C-(Ct)2(O)2							C-(H)2(CO)(CCO)						
C-(CO)2(O)2					[3]	[12]							
C-(C)(Cb)(O)2							C-(C)3(CO)	1.4	5.9	3.5	14.6	-5.2	-21.8
C-(C)(Cd)(O)2							C-(C)2(CO)2	1.6	6.7			10.3	43.1
C-(C)(Ct)(O)2							C-(Cb)2(CO)2						
C-(Cb)(Cd)(O)2							C-(Cd)2(CO)2						
C-(Cb)(Ct)(O)2							C-(Cb)(Cd)(CO)2						
C-(Cd)(Ct)(O)2							C-(Cb)(Ct)(CO)2						
C-(C)(O)2(CO)							C-(C)(Cb)(CO)2						
C-(Cb)(O)2(CO)													
C-(Cd)(O)2(CO)							C-(H)3(CO)	-10.0	-41.8	-11.6	-48.5	-10.1	-42.3
C-(Ct)(O)2(CO)							C-(CCO)(H)3	-10.0	-41.8	-11.6	-48.5	-10.1	-42.3

Table 2. Comparison of group additivity values, Enthalpy of formation (298 K), 3

Group	Group Additivity Value						Group	Group Additivity Value					
	Gas		Liquid		Solid			Gas		Liquid		Solid	
	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol		kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol
Cd-(H)(O)	8.6	36.0	7.0	29.3	0.0	0.0	O-(H)2	-57.8	-241.8	-68.3	-285.8	-69.7	-291.8
Cd-(H)(CO)	5.2	21.8	2.0	8.4	6.0	25.1							
Cd-(H)(CCO)							O-(C)(H)	-37.9	-158.6	-45.5	-190.4	-50.0	-209.2
							O-(Cb)(H)	-38.5	-161.1	-46.6	-195.0	-46.7	-195.4
Cd-(C)(O)	8.9	37.2	5.0	20.9	4.0	16.7	O-(Cd)(H)	-49.3	-206.3	-51.0	-213.4	-52.4	-219.2
Cd-(Cb)(O)	10.4	43.5			1.2	5.0	O-(Ct)(H)	[37.9]	[158.6]				
Cd-(Cd)(O)	9.5	39.7	9.0	37.7	9.0	37.7	O-(H)(CO)	-57.8	-241.8	-66.2	-277.0	-61.4	-256.9
Cd-(Ct)(O)	7.6	31.8					O-(H)(CCO)						
Cd-(O)(CO)	11.6	48.5	6.0	25.1	8.0	33.5							
							O-(C)2	-23.6	-99.6	-25.1	-105.0	-25.0	-104.6
Cd-(C)(CO)	7.5	31.4	9.8	41.0	7.8	32.6	O-(C)(Cb)	-21.6	-90.4	-25.0	-104.6	-32.2	-134.7
Cd-(Cb)(CO)	8.0	33.5			8.0	33.5	O-(C)(Cd)	-30.5	-127.6	-31.0	-129.7	-31.0	-129.7
Cd-(Cd)(CO)	8.3	34.7	1.9	7.9			O-(C)(Ct)						
Cd-(Ct)(CO)							O-(C)(CO)	-43.1	-180.3	-44.5	-186.2	-44.0	-184.1
Cd-(CO)2	13.3	55.6			[27]	[113]	O-(Cb)2	-18.9	-79.1	-20.4	-85.4	-19.0	-79.5
Cd-(CCO)(CO)							O-(Cb)(Cd)	-21.0	-87.9	-26.6	-111.3		
							O-(Cb)(Ct)						
Cb-(O)	-0.9	-3.8	-1.4	-5.9	-1.0	-4.2	O-(Cd)2	-33.0	-138.1	-33.0	-138.1	-33.0	-138.1
Cb-(CO)	3.7	15.5	4.2	17.6	4.5	18.8	O-(Cd)(Ct)						
Cb-(CCO)	4.0	16.7					O-(Ct)2						
							O-(Cb)(CO)	-36.7	-153.6	-37.0	-154.8	-35.0	-146.4
Ct-(O)	[31.9]	[133.5]					O-(Cd)(CO)	-44.8	-187.4	-45.0	-188.3		
Ct-(CO)	28.4	118.8	29.0	121.3	25.6	107.1	O-(Ct)(CO)						
Ct-(CCO)							O-(CO)2	-46.2	-193.3	-53.0	-221.8	-51.0	-213.4
							O-(C)(CCO)						
CO-(C)(H)	-29.4	-123.0	-34.3	-143.5			O-(Cb)(CCO)						
CO-(Cb)(H)	-29.1	-121.8	-35.0	-146.4	-29.8	-124.7	O-(Cd)(CCO)						
CO-(Cd)(H)	-27.6	-115.5	-30.0	-125.5	-35.1	-146.9	O-(Ct)(CCO)						
CO-(Ct)(H)													
CO-(H)(CO)	-25.2	-105.4	-32.3	-135.1	-41.0	-171.5	O-(H)(O)	-16.3	-68.2	-22.8	-95.4	-23.9	-100.2
CO-(H)(O)	-31.9	-133.5	-36.2	-151.5			O-(C)(O)	-5.0	-20.9	-6.2	-25.9	-11.0	-46.0
CO-(C)(O)	-35.2	-147.3	-38.1	-159.4	-35.5	-148.5	O-(Cb)(O)	[-5]	[-21]			-4.5	-18.8
CO-(Cb)(O)	-34.4	-143.9	-36.9	-154.4	-40.8	-170.7	O-(Cd)(O)						
CO-(Cd)(O)	-32.2	-134.7	-32.7	-136.8	-39.0	-163.2	O-(Ct)(O)						
CO-(Ct)(O)	-39.5	-165.3	-35.2	-147.3	-34.1	-142.7	O-(O)(CO)	-18.2	-76.1	-20.8	-87.0	-15.4	-64.4
CO-(O)(CO)	-29.5	-123.4	-31.7	-132.6	-36.0	-150.6	O-(O)(CCO)						
CO-(O)2	-29.9	-125.1	-30.0	-125.5	-33.0	-138.1	O-(O)2	14.7	61.5	[13.4]	[56.1]		
CO-(C)2	-31.7	-132.6	-36.2	-151.5	-35.4	-148.1							
CO-(Cb)2	-27.0	-113.0	-28.0	-117.2	-33.5	-140.2	CCO-(H)2	-11.4	-47.7	-16.2	-67.8		
CO-(Cd)2	-30.0	-125.5	-31.0	-129.7	-39.0	-163.2	CCO-(C)(H)	-15.0	-62.8				
CO-(Ct)2							CCO-(Cb)(H)	25.6	107.1				
CO-(C)(Cb)	-30.9	-129.3	-37.0	-154.8	-39.5	-165.3	CCO-(Cd(H)						
CO-(C)(Cd)	-32.4	-135.6	-32.0	-133.9	-27.0	-113.0	CCO-(Ct)(H)						
CO-(C)(Ct)	-30.0	-125.5	[-42]	[-176]									
CO-(Cb)(Cd)	-39.8	-166.5			-31.9	-133.5	CCO-(C)2	-12.0	-50.2				
CO-(Cb)(Ct)							CCO-(Cb)2	-15.8	-66.1				
CO-(C)(CO)	-30.2	-126.4	-32.1	-134.3	-21.8	-91.2	CCO-(Cd)2						
CO-(Cb)(CO)	-26.5	-110.9			-30.4	-127.2	CCO-(Ct)2						
CO-(Cd)(CO)	-28.3	-118.4	-28.1	-117.6	-28.0	-117.2	CCO-(CO)2						
CO-(Ct)(CO)													

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 1

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
Methane	CH4 (1)	74-82-8	-74.4											
Ethyne	C2H2 (1)	74-86-2	228.2		227.6	0.6	206.3	a	217.6	-11.3				
Ethene	C2H4 (1)	74-85-1	52.5		52.7	-0.2								
Ethane	C2H6 (1)	74-84-0	-83.8		-83.7	-0.1	-93.7	P94	-97.1	3.3				
Propyne	C3H4 (1)	74-99-7	184.9		186.2	-1.3								
Allene	C3H4 (2)	463-49-0	190.5		195.8	-5.3								
Cyclopropene	C3H4 (3)	2781-85-3	277.1		278.2	-1.1								
Propene	C3H6 (1)	115-07-1	20.0		20.5	-0.5	1.7		4.2	-2.5				
Cyclopropane	C3H6 (2)	75-19-4	53.3		53.1	0.2	35.1	P94	36.4	-1.3				
Propane	C3H8 (1)	74-98-6	-104.7		-104.6	-0.1	-120.9	P94	-122.6	1.7				
1-Buten-3-yne	C4H4		304.6	SWS	284.9	19.7								
1-Butyne	C4H6 (1)	107-00-6	165.2		166.5	-1.3	141.9		144.8	-2.9				
2-Butyne	C4H6 (2)	503-17-3	145.7		144.8	0.9	119.1		116.3	2.8				
1,2-Butadiene	C4H6 (3)	590-19-2	162.3		163.6	-1.3	139.0		141.0	-2.0				
1,3-Butadiene	C4H6 (4)	106-99-0	110.0		109.6	0.4	87.9		85.4	2.5				
Cyclobutene	C4H6 (5)	822-35-5	156.7		156.5	0.2								
Methylenecyclopropane	C4H6 (6)	6142-73-0	200.5		200.4	0.1								
1-Methylcyclopropene	C4H6 (7)	3100-04-7	243.6		243.1	0.5								
Bicyclo[1.1.0]butane	C4H6 (8)	157-33-5	217.1		218.4	-1.3	193.7		190.0	3.7				
1-Butene	C4H8 (1)	106-98-9	0.1		0.4	-0.3	-20.5		-21.3	0.8				
(Z)-2-Butene	C4H8 (2)	590-18-1	-7.1		-7.1	0.0	-29.7		-28.9	-0.8				
(E)-2-Butene	C4H8 (3)	624-64-6	-11.4		-11.7	0.3	-33.0		-32.6	-0.4				
2-Methylpropene	C4H8 (4)	115-11-7	-16.9		-14.6	-2.3	-37.5		-36.0	-1.5				
Cyclobutane	C4H8 (5)	287-23-0	28.4		28.5	-0.1	3.7		3.8	-0.1				
Methylcyclopropane	C4H8 (6)	594-11-6					1.7		-12.1	13.8				
Butane	C4H10 (1)	106-97-8	-125.6		-125.5	-0.1	-146.6		-148.1	1.5				
2-Methylpropane (Isobutane)	C4H10 (2)	75-28-5	-134.2		-135.6	1.4	-153.5		-154.8	1.3				
(Z)-3-Penten-1-yne	C5H6 (1)	1574-40-9	255.1	b	249.8	5.3	226.5		226.8	-0.3				
(E)-3-Penten-1-yne	C5H6 (2)	2004-69-5	257.7	b	252.7	5.0	228.2		229.3	-1.1				
1,3-Cyclopentadiene	C5H6 (3)	542-92-7	134.3		134.7	-0.4	105.9		106.3	-0.4				
2-Methyl-1-buten-3-yne	C5H6	78-80-8	258.6	c	254.8	3.8								
1,2-Pentadiene	C5H8 (1)	591-95-7	140.7		143.5	-2.8								
(Z)-1,3-Pentadiene	C5H8 (2)	1574-41-0	81.4		82.0	-0.6								
(E)-1,3-Pentadiene	C5H8 (3)	2004-70-8	76.1		77.4	-1.3								
1,4-Pentadiene	C5H8 (4)	591-93-5	105.6		106.7	-1.1	81.2	DH	81.2	-0.0				
2,3-Pentadiene	C5H8 (5)	591-96-8	133.1		131.4	1.7	105.6	DH	104.2	1.4				
2-Methyl-1,3-butadiene (Isoprene)	C5H8 (6)	78-79-5	75.5		76.1	-0.6	48.2		48.1	0.1				
Cyclopentene	C5H8 (7)	142-29-0	33.9		35.6	-1.7	4.4		7.5	-3.1				
Ethenylcyclopropane (Vinylcyclopropane)	C5H8 (8)	693-86-7					122.5		105.4	17.1				
Spiropentane	C5H8 (9)	157-40-4	185.2		185.4	-0.2	157.7		158.2	-0.5				
3-Methyl-1,2-butadiene	C5H8 (10)	598-25-4	128.9	d	128.4	0.4	101.2	d	100.8	0.4				
Methylenecyclobutane	C5H8 (11)	1120-56-5	121.5		121.8	-0.3	93.8		93.3	0.5				

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 2

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
1-Pentyne	C5H8	627-19-0	144.2	b	145.6	-1.4	116.0	b	119.2	-3.2				
2-Pentyne	C5H8	627-21-4	124.6	b	125.1	-0.5	94.3	b	94.1	0.1				
3-Methyl-1-butyne	C5H8	598-23-2	136.9	b	136.8	0.1	110.2	b	110.0	0.1				
1-Pentene	C5H10 (1)	109-67-1	-21.3		-20.5	-0.8	-46.9		-46.9	-0.0				
(Z)-2-Pentene	C5H10 (2)	627-20-3	-27.6		-27.2	-0.4	-53.7		-54.4	0.7				
(E)-2-Pentene	C5H10 (3)	646-04-8	-31.9		-31.8	-0.1	-58.2		-58.2	-0.0				
2-Methyl-1-butene	C5H10 (4)	563-46-2	-35.3		-34.7	-0.6	-61.0		-61.5	0.5				
3-Methyl-1-butene	C5H10 (5)	563-45-1	-27.6		-28.5	0.9	-51.5		-54.4	2.9				
2-Methyl-2-butene	C5H10 (6)	513-35-9	-41.8		-42.3	0.5	-68.6		-69.0	0.4				
Ethylcyclopropane	C5H10 (7)	1191-96-4					-24.8		-37.7	12.9				
Methylcyclobutane	C5H10 (8)	598-61-8	-20.9	SWS	-13.4	-7.5	-44.5		-44.8	0.3				
Cyclopentane	C5H10 (9)	287-92-3	-76.4		-74.9	-1.5	-105.1		-105.0	-0.1				
(Z)-1,2-Dimethylcyclopropane	C5H10 (10)	930-18-7					-26.3		-18.8	-7.5				
(E)-1,2-Dimethylcyclopropane	C5H10 (11)	2402-06-4					-30.7		-18.8	-11.9				
1,1-Dimethylcyclopropane	C5H10 (13)	1630-94-0	-8.2		-10.0	1.8	-33.3		-31.8	-1.5				
Pentane	C5H12 (1)	109-66-0	-146.9		-146.4	-0.5	-173.5		-173.6	0.1				
2-Methylbutane (Isopentane)	C5H12 (2)	78-78-4	-153.7		-153.1	-0.6	-178.5		-178.0	-0.5				
2,2-Dimethylpropane	C5H12 (3)	463-82-1	-168.1		-167.8	-0.3	-190.2		-190.8	0.6				
1,5-Hexadiyne	C6H6 (1)	628-16-0	418.6	b	416.7	1.9	384.2		386.6	-2.4				
Benzene	C6H6 (2)	71-43-2	82.6		82.8	-0.2	49.0		49.2	-0.2				
2,4-Hexadiyne	C6H6		330.5	SWS	356.5	-25.9								
3,4-Dimethylenecyclo-1-butene	C6H6	5291-90-7	336.4	e	289.5	46.9								
Fulvene (5-Methylene-1,3-cyclopentadiene)	C6H6	497-20-1	223.8	f	209.6	14.2								
1,3-Cyclohexadiene	C6H8 (1)	592-57-4	106.2		105.4	0.8	73.2		74.5	-1.3				
1,4-Cyclohexadiene	C6H8 (2)	628-41-1	100.4	P94	95.4	5.0	66.1	P94	66.1	0.0				
Bicyclo[2.2.0]-2-hexene	C6H8	3097-63-8					228.0	g	228.0					
1,5-Hexadiene	C6H10 (1)	592-42-7	84.1		84.5	-0.4	54.1		54.4	-0.3				
2,3-Dimethyl-1,3-butadiene	C6H10 (2)	513-81-5	45.1		42.7	2.4	14.1		10.9	3.2				
1-Methylcyclopentene	C6H10 (3)	693-89-0	-3.8		0.4	-4.2	-36.4		-32.6	-3.8				
3-Methylcyclopentene	C6H10 (4)	1120-62-3	7.4		6.7	0.7	-23.7		-25.5	1.8				
4-Methylcyclopentene	C6H10 (5)	1759-81-5	14.6		4.6	10.0	-17.6		-24.7	7.1				
Cyclohexene	C6H10 (6)	110-83-8	-5.0		-7.9	2.9	-38.5		-41.0	2.5				
Bicyclopropyl	C6H10 (7)	5685-46-1	129.4		128.0	1.4	95.9		105.4	-9.5				
Methylenecyclopentane	C6H10 (8)	1528-30-9	12.0		16.7	-4.7	-20.1		-18.4	-1.7				
Bicyclo[3.1.0]hexane	C6H10 (9)	285-58-5	38.3		36.0	2.3	5.1		4.2	0.9				
3,3-Dimethyl-1-butyne	C6H10 (10)	917-92-0	106.4	b	107.9	-1.6	78.4		77.8	0.6				
1-Hexyne	C6H10	693-02-7	122.3	h	124.7	-2.4	90.7	h	93.7	-3.1				
2-Hexyne	C6H10	764-35-2	107.7	h	104.2	3.5	76.0	h	68.6	7.4				
3-Hexyne	C6H10	928-49-4	105.4	h	105.4	-0.0	73.7	h	72.0	1.8				
2-Cyclopropylpropene	C6H10						49.0	SWS	64.4	-15.5				
Dimethylmethylenecyclopropane	C6H10						-32.2	SWS	-32.6	0.4				
1-Hexene	C6H12 (1)	592-41-6	-41.4	DH	-41.4		-74.2		-72.4	-1.8				

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 3

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
(Z)-2-Hexene	C6H12 (2)	7688-21-3	-47.7	L	-48.1	0.4	-83.9		-79.9	-4.0				
(E)-2-Hexene	C6H12 (3)	4050-45-7	-53.9		-52.7	-1.2	-85.5		-83.7	-1.8				
(Z)-3-Hexene	C6H12 (4)	7642-09-3	-47.6		-47.3	-0.3	-79.0		-79.9	0.9				
(E)-3-Hexene	C6H12 (5)	13269-52-8	-54.4		-51.9	-2.5	-86.1		-83.7	-2.4				
2-Methyl-1-pentene	C6H12 (6)	763-29-1	-57.3	i	-55.6	-1.7	-90.0		-87.0	-3.0				
3-Methyl-1-pentene	C6H12 (7)	760-20-3	-49.5		-49.4	-0.1	-78.2		-79.9	1.7				
4-Methyl-1-pentene	C6H12 (8)	691-37-2	-49.4	i	-48.1	-1.3	-80.0		-76.8	-3.2				
2-Methyl-2-pentene	C6H12 (9)	625-27-4	-64.9	i	-62.3	-2.5	-98.5		-94.6	-3.9				
(Z)-3-Methyl-2-pentene	C6H12 (10)	922-62-3	-62.3		-62.3	0.0	-94.5		-94.6	0.1				
(E)-3-Methyl-2-pentene	C6H12 (11)	616-12-6	-63.1		-62.3	-0.8	-94.6		-94.6	-0.0				
(Z)-4-Methyl-2-pentene	C6H12 (12)	691-38-3	-57.5		-56.1	-1.4	-87.0		-87.4	0.4				
(E)-4-Methyl-2-pentene	C6H12 (13)	674-76-0	-61.5		-60.7	-0.8	-91.5		-91.2	-0.3				
2-Ethyl-1-butene	C6H12 (14)	760-21-4	-56.0		-54.8	-1.2	-87.1		-87.0	-0.1				
2,3-Dimethyl-1-butene	C6H12 (15)	563-78-0	-62.6		-60.2	-2.4	-93.3		-90.4	-2.9				
3,3-Dimethyl-1-butene	C6H12 (16)	558-37-2	-60.5		-56.1	-4.4	-87.6		-83.3	-4.3				
2,3-Dimethyl-2-butene (Tetramethylethylene)	C6H12 (17)	563-79-1	-68.2		-68.2	-0.0	-101.5		-101.7	0.2				
Methylcyclopentane	C6H12 (18)	96-37-7	-106.2		-105.9	-0.3	-137.9		-137.2	-0.7				
Cyclohexane	C6H12 (19)	110-82-7	-123.4		-122.6	-0.8	-156.4		-156.1	-0.3				
1,1,2-Trimethylcyclopropane	C6H12 (20)	4127-45-1					-96.2		-64.0	-32.2				
Ethylcyclobutane	C6H12 (21)	4806-61-5	-26.3		-23.4	-2.9	-59.0		-54.0	-5.0				
Hexane	C6H14 (1)	110-54-3	-167.1		-167.4	0.3	-198.7		-199.2	0.5				
2-Methylpentane	C6H14 (2)	107-83-5	-174.8		-174.1	-0.7	-204.6		-203.6	-1.0				
3-Methylpentane	C6H14 (3)	96-14-0	-172.1		-170.7	-1.4	-202.4		-201.3	-1.1				
2,3-Dimethylbutane	C6H14 (4)	79-29-8	-178.3		-180.7	2.4	-207.4		-207.9	0.5				
2,2-Dimethylbutane	C6H14 (5)	75-83-2	-186.1		-182.0	-4.1	-213.8		-211.7	-2.1				
Benzocyclopropene	C7H6	4646-69-9	372.4	j	370.7	1.7								
1,3,5-Cycloheptatriene	C7H8 (1)	544-25-2	180.9		182.0	-1.1	142.2		142.7	-0.5				
Toluene	C7H8 (2)	108-88-3	50.4		50.2	0.2	12.4		12.6	-0.2				
Bicyclo[2.2.1]hepta-2,5-diene (Norbornadiene)	C7H8 (4)	121-46-0	245.9		246.9	-1.0	213.0		213.8	-0.8				
3,3-Dimethyl-1,4-pentadiyne	C7H8 (5)	62496-43-9					348.7		348.5	0.2				
3-Methylene-1,4-cyclohexadiene	C7H8	3217-87-6	146.4	k	152.3	-5.9								
5-Methylene-1,3-cyclohexadiene	C7H8	20679-59-8	171.5	k	183.3	-11.7								
3-Methylenecyclohexene	C7H10 (1)	1888-90-0					-12.7		28.5	-41.2				
2-Methyl-1,3-cyclohexadiene	C7H10 (2)	1489-57-2					-58.7		37.2	-95.9				
1,3-Cycloheptadiene	C7H10 (3)	4054-38-0	94.3		95.0	-0.7	52.3	l	52.7	-0.4				
Bicyclo[2.2.1]hept-2-ene (Norbornene)	C7H10 (5)	498-66-8	90.0		90.4	-0.4					52.9		53.1	-0.2
1,4-Cycloheptadiene	C7H10	7161-35-5					77.4	l	78.2	-0.8				
1-Ethylcyclopentene	C7H12 (1)	2146-38-5	-19.7		-19.7	-0.0	-58.3		-58.2	-0.1				
Ethenylcyclopentane (Vinylcyclopentane)	C7H12 (2)	3742-34-5					-34.8		-36.8	2.0				
Ethylidenecyclopentane	C7H12 (3)	2146-37-4	-18.1		-15.5	-2.6	-56.7		-55.2	-1.5				
1-Methylcyclohexene	C7H12 (4)	591-49-1	-43.3		-43.1	-0.2	-81.2		-81.2	-0.0				
Methylenecyclohexane	C7H12 (5)	1192-37-6	-25.2		-31.0	5.8	-61.3		-69.5	8.2				

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 4

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
Cycloheptene	C7H12 (6)	628-92-2	-9.2		-8.4	-0.8								
Bicyclo[4.1.0]heptane	C7H12 (7)	286-08-8	1.5		1.7	-0.2	-36.7		-36.4	-0.3				
Bicyclo[2.2.1]heptane (Norbornane)	C7H12 (8)	279-23-2	-54.9		-57.7	2.8					-95.1		-96.2	1.1
1-Methyl-bicyclo[3.1.0]-hexane	C7H12 (9)	4625-24-5	1.5		3.8	-2.3	-33.2		-31.8	-1.4				
1,2-Dimethylcyclopentene	C7H12		-41.4	m	-30.1	-11.3								
1-Heptyne	C7H12	628-71-7	103.8	h	103.8	0.0	67.2	h	68.2	-1.0				
2-Heptyne	C7H12	1119-65-9	84.8	h	83.3	1.5	48.2	h	43.1	5.1				
3-Heptyne	C7H12	2586-89-2	82.8	h	84.5	-1.8	46.2	h	46.4	-0.3				
2-Cyclopropyl-1-butene	C7H12						83.3	SWS	38.9	44.4				
2-Cyclopropyl-2-butene	C7H12						62.3	SWS	27.6	34.7				
4-Methylcyclohexene	C7H12						-102.1	SWS	-72.8	-29.3				
1-Heptene	C7H14 (1)	592-76-7	-62.3		-62.3	0.0	-97.9		-97.9	0.0				
5-Methyl-1-hexene	C7H14 (2)	3524-73-0	-65.7		-69.0	3.3	-100.0		-102.3	2.3				
(Z)-3-Methyl-3-hexene	C7H14 (3)	4914-89-0	-79.4		-82.4	3.0	-115.9		-120.1	4.2				
(E)-3-Methyl-3-hexene	C7H14 (4)	3899-36-3	-76.8		-82.4	5.6	-112.7		-120.1	7.4				
2,4-Dimethyl-1-pentene	C7H14 (5)	2213-32-3	-83.8		-83.3	-0.5	-117.0		-116.9	-0.1				
4,4-Dimethyl-1-pentene	C7H14 (6)	762-62-9	-81.6		-77.0	-4.6	-110.6		-110.5	-0.1				
2,4-Dimethyl-2-pentene	C7H14 (7)	625-65-0	-88.7		-87.9	-0.8	-123.1		-123.4	0.3				
(Z)-4,4-Dimethyl-2-pentene	C7H14 (8)	762-63-0	-72.6		-69.9	-2.7	-105.3		-105.0	-0.3				
(E)-4,4-Dimethyl-2-pentene	C7H14 (9)	690-08-4	-88.8		-88.3	-0.5	-121.7		-120.1	-1.6				
3-Methyl-2-ethyl-1-butene	C7H14 (10)	7357-93-9	-79.5		-80.3	0.8	-114.1		-115.9	1.8				
2,3,3-Trimethyl-1-butene	C7H14 (11)	594-56-9	-85.5		-87.9	2.4	-117.7		-119.2	1.5				
1,1-Dimethyl-2-ethylcyclopropane	C7H14 (12)	41845-47-0					-90.2		-89.5	-0.7				
1,1-Dimethylcyclopentane	C7H14 (13)	1638-26-2	-138.2		-138.1	-0.1	-172.0		-173.2	1.2				
(Z)-1,2-Dimethylcyclopentane	C7H14 (14)	1192-18-3	-129.5		-136.8	7.3	-165.3		-169.5	4.2				
(E)-1,2-Dimethylcyclopentane	C7H14 (15)	822-50-4	-136.6		-136.8	0.2	-171.2		-169.5	-1.7				
(Z)-1,3-Dimethylcyclopentane	C7H14 (16)	2532-58-3	-135.9		-136.8	0.9	-170.1		-169.5	-0.6				
(E)-1,3-Dimethylcyclopentane	C7H14 (17)	1759-58-6	-133.6		-136.8	3.2	-168.1		-169.5	1.4				
Ethylcyclopentane	C7H14 (18)	1640-89-7	-126.9		-126.8	-0.1	-163.4		-162.8	-0.6				
Methylcyclohexane	C7H14 (19)	108-87-2	-154.7		-153.6	-1.1	-190.1		-188.3	-1.8				
Cycloheptane	C7H14 (20)	291-64-5	-118.1		-118.0	-0.1	-156.6		-156.5	-0.1				
1,1,2,2-Tetramethylcyclopropane	C7H14 (21)	4127-47-3					-119.7		-100.0	-19.7				
(Z)-1,2-Diethylcyclopropane	C7H14 (22)	71032-67-2					-79.9		-79.1	-0.8				
(E)-1,2-Diethylcyclopropane	C7H14 (23)	71032-66-1					-83.3		-79.1	-4.2				
(Z)-2-Heptene	C7H14 (24)	6443-92-1					-105.1		-105.4	0.3				
(E)-2-Heptene	C7H14 (25)	14686-13-6					-109.5		-109.2	-0.3				
(Z)-3-Heptene	C7H14 (26)	7642-10-6					-104.3		-105.4	1.1				
(E)-3-Heptene	C7H14 (27)	14686-14-7					-109.3		-109.2	-0.1				
2,3-Dimethyl-1-pentene	C7H14						-119.6	n	-120.1	0.5				
3,3-Dimethyl-1-pentene	C7H14						-111.3	n	-108.8	-2.5				
3,4-Dimethyl-1-pentene	C7H14						-111.3	n	-112.1	0.8				
2,3-Dimethyl-2-pentene	C7H14	10574-37-5					-126.7	n	-127.2	0.5				

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 5

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
(Z)-3,4-Dimethyl-2-pentene	C7H14						-124.8	n	-123.4	-1.4				
(E)-3,4-Dimethyl-2-pentene	C7H14						-125.1	n	-123.4	-1.7				
2-Ethyl-1-pentene	C7H14						-111.8	n	-112.5	0.8				
3-Ethyl-1-pentene	C7H14						-104.2	n	-105.4	1.3				
3-Ethyl-2-pentene	C7H14						-118.0	n	-120.1	2.1				
Heptane	C7H16 (1)	142-82-5	-187.7		-188.3	0.6	-224.2		-224.7	0.5				
2-Methylhexane (Isoheptane)	C7H16 (2)	591-76-4	-194.6		-195.0	0.4	-229.5		-229.1	-0.4				
3-Methylhexane	C7H16 (3)	589-34-4	-191.3		-191.6	0.3	-226.4		-226.8	0.4				
3-Ethylpentane	C7H16 (4)	617-78-7	-189.6		-188.3	-1.3	-224.8		-224.5	-0.3				
2,2-Dimethylpentane	C7H16 (5)	590-35-2	-205.9		-202.9	-3.0	-238.3		-237.2	-1.1				
2,3-Dimethylpentane	C7H16 (6)	565-59-3	-198.9		-198.3	-0.6	-233.1		-231.2	-1.9				
2,4-Dimethylpentane	C7H16 (7)	108-08-7	-201.7		-201.7	-0.0	-234.6		-233.5	-1.1				
3,3-Dimethylpentane	C7H16 (8)	562-49-2	-201.2		-196.2	-5.0	-234.2		-232.6	-1.6				
2,2,3-Trimethylbutane	C7H16 (9)	464-06-2	-204.5		-206.3	1.8	-236.5		-239.3	2.8				
Phenylacetylene (Ethynylbenzene)	C8H6 (1)	536-74-3	305.4	L	309.6	-4.2	283.5		283.7	-0.2				
1,2-Cyclobutylbenzene	C8H8	694-87-1	200.8	o	201.3	-0.4								
1,3,5,7-Cyclooctatetraene	C8H8 (1)	629-20-9	295.9		296.6	-0.7	254.5		254.4	0.1				
Styrene (Ethenylbenzene)	C8H8 (3)	100-42-5	147.9		148.1	-0.2	103.8		101.3	2.5				
3,6-bis(methylene)-1,4-cyclohexadene	C8H8	502-86-3	209.2	p	209.2									
5,6-bis(methylene)-1,3-cyclohexadene	C8H8		221.8	p	238.5	-16.7								
1,7-Octadiyne	C8H10 (1)	871-84-1	376.1	b	374.9	1.2	334.4		335.6	-1.2				
Ethylbenzene	C8H10 (2)	100-41-4	29.9		31.0	-1.1	-12.3		-13.4	1.1				
o-Xylene (1,2-Dimethylbenzene)	C8H10 (3)	95-47-6	19.1		20.1	-1.0	-24.4		-22.4	-2.0				
m-Xylene (1,3-Dimethylbenzene)	C8H10 (4)	108-38-3	17.3		17.6	-0.3	-25.4		-24.1	-1.3				
p-Xylene (1,4-Dimethylbenzene)	C8H10 (5)	106-42-3	18.0		17.6	0.4	-24.4		-24.1	-0.3				
5-Isopropylidenecyclopentadiene	C8H10 (6)	2175-91-9	134.4		156.1	-21.7	90.0		89.5	0.5				
1-Octen-3-yne	C8H12 (1)	17679-92-4	181.9	b	182.0	-0.1	140.7		142.3	-1.6				
Bicyclo[2.2.2]-2-octene	C8H12 (2)	931-64-6	20.5		18.4	2.1					-23.3		-23.0	-0.3
2-Methylenebicyclo[2.2.1]-heptane	C8H12 (3)	497-35-8					-4.1		6.7	-10.8				
endo-5-Methylbicyclo[2.2.1]-2-heptene	C8H12 (4)	10060-47-6					15.8		2.5	13.3				
(Z)-1,2-Diethenylcyclobutane	C8H12 (6)	16177-46-1	166.5		184.1	-17.6	124.3		142.5	-18.2				
(E)-1,2-Diethenylcyclobutane	C8H12 (7)	6553-48-6	143.5		180.7	-37.2	101.3		140.2	-38.9				
4-Ethenylcyclohexene	C8H12 (8)	100-40-3	65.1		68.2	-3.1	26.8		27.2	-0.4				
(Z,Z)-1,5-Cyclooctadiene	C8H12 (9)	1552-12-1	101.1		101.3	-0.2	57.7		58.6	-0.9				
2-Methylbicyclo[2.2.1]-2-heptene	C8H12 (10)	694-92-8					4.5		-5.4	9.9				
7-Methylenebicyclo[2.2.1]-heptane	C8H12 (11)	31463-35-1	60.2		38.1	22.1	19.7		5.9	13.8				
1-Methyl-3-methylene-1-cyclohexene	C8H12						-45.6	SWS	-46.0	0.4				
3-Cyclopentylpropene	C8H14 (1)	3524-75-2	-24.1		-21.8	-2.3	-64.5		-61.5	-3.0				
1-Ethylcyclohexene	C8H14 (2)	1453-24-3	-63.4		-63.2	-0.2	-106.7		-106.7	-0.0				
Ethylidenecyclohexane	C8H14 (3)	1003-64-1	-61.5		-63.2	1.7	-103.5		-106.3	2.8				
Ethenylcyclohexane	C8H14 (4)	695-12-5	-48.9		-49.4	0.5	-88.7		-87.0	-1.7				
(Z)-Cyclooctene	C8H14 (5)	931-88-4	-27.0		-26.8	-0.2	-74.0		-73.6	-0.4				

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 6

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
(E)-Cyclooctene	C8H14						-32.9	q	-32.2	-0.7				
Bicyclo[4.2.0]octane	C8H14 (6)	278-30-8	-26.2		-26.4	0.2	-68.1		-67.8	-0.3				
Bicyclo[5.1.0]octane	C8H14 (7)	286-43-1	-16.6		-16.7	0.1	-60.2		-59.8	-0.4				
(Z)-Bicyclo[3.3.0]octane (Octahydropentalene)	C8H14 (8)	1755-05-1	-92.9		-92.9	-0.0	-136.0		-136.2	0.2				
(E)-Bicyclo[3.3.0]octane	C8H14 (9)	5597-89-7	-66.6		-66.5	-0.1	-109.2		-109.0	-0.2				
Bicyclo[2.2.2]octane	C8H14 (10)	280-33-1	-99.0		-101.3	2.3	-146.9		-138.1	-8.8				
1-Methylbicyclo[4.1.0]heptane	C8H14 (14)	2439-79-4	-20.8		-30.5	9.7	-59.9		-72.4	12.5				
1-Octyne	C8H14	629-05-0	80.7	h	82.8	-2.1	39.2	h	42.7	-3.5				
2-Octyne	C8H14	2809-67-8	63.8	h	62.3	1.4	39.0	h	17.6	21.4				
3-Octyne	C8H14	15232-76-5	62.5	h	63.6	-1.1	21.0	h	20.9	0.1				
4-Octyne	C8H14	1942-45-6	60.1	h	63.6	-3.5	18.6	h	20.9	-2.3				
2,5-Dimethyl-2,4-hexadiene	C8H14	764-13-6	-19.2	d	-25.1	5.9	-63.2	d	-68.6	5.4				
2-Cyclopropyl-3-methyl-1-butene	C8H14						12.6	SWS	5.9	6.7				
2-Cyclopropyl-1-pentene	C8H14						-29.3	SWS	5.0	-34.3				
2-Cyclopropyl-2-pentene	C8H14						-8.4	SWS	2.1	-10.5				
2,4-Dimethylcyclohexene	C8H14						-149.8	SWS	-113.4	-36.4				
1,2,3-Trimethylcyclopentene	C8H14						-158.6	SWS	-105.9	-52.7				
2,3,3-Trimethylcyclopentene	C8H14						-157.3	SWS	-94.6	-62.8				
1-Octene	C8H16 (1)	111-66-0	-82.8	DH	-83.3	0.4	-124.5	r	-123.4	-1.1				
(Z)-2,2-Dimethyl-3-hexene	C8H16 (2)	690-92-6	-89.3		-90.0	0.7	-126.4		-130.5	4.1				
(E)-2,2-Dimethyl-3-hexene	C8H16 (3)	690-93-7	-107.7		-108.4	0.7	-144.9		-145.6	0.7				
2-Methyl-3-ethyl-1-pentene	C8H16 (4)	19780-66-6	-100.3		-102.1	1.8	-137.9		-141.4	3.5				
2,4,4-Trimethyl-1-pentene	C8H16 (5)	107-39-1	-110.6		-112.1	1.5	-145.9		-146.6	0.7				
2,4,4-Trimethyl-2-pentene	C8H16 (6)	107-40-4	-104.9		-105.0	0.1	-142.4		-145.2	2.8				
1,1-Dimethyl-2-propylcyclopropane	C8H16 (7)	41845-48-1					-116.0		-115.1	-0.9				
Propylcyclopentane	C8H16 (8)	2040-96-2	-147.7		-147.7	-0.0	-188.8		-188.3	-0.5				
Ethylcyclohexane	C8H16 (9)	1678-91-7	-171.7		-174.5	2.8	-211.9		-213.8	1.9				
1,1-Dimethylcyclohexane	C8H16 (10)	590-66-9	-180.9		-184.5	3.6	-218.7		-220.5	1.8				
(Z)-1,2-Dimethylcyclohexane	C8H16 (11)	2207-01-4	-172.1		-174.5	2.4	-211.8		-213.6	1.8				
(E)-1,2-Dimethylcyclohexane	C8H16 (12)	6876-23-9	-179.9		-181.2	1.3	-218.2		-218.2	-0.0				
(Z)-1,3-Dimethylcyclohexane	C8H16 (13)	638-04-0	-184.6		-184.5	-0.1	-222.9		-220.5	-2.4				
(E)-1,3-Dimethylcyclohexane	C8H16 (14)	2207-03-6	-176.5		-177.8	1.3	-215.7		-215.9	0.2				
(Z)-1,4-Dimethylcyclohexane	C8H16 (15)	624-29-3	-176.6		-177.8	1.2	-215.6		-215.9	0.3				
(E)-1,4-Dimethylcyclohexane	C8H16 (16)	2207-04-7	-184.5		-184.5	0.0	-222.4		-220.5	-1.9				
Cyclooctane	C8H16 (17)	292-64-8	-124.4		-124.3	-0.1	-167.7		-167.4	-0.3				
(Z)-2-Octene	C8H16 (18)	7642-04-8					-130.7	r	-131.0	0.3				
(E)-2-Octene	C8H16 (19)	13389-42-9					-134.6	r	-134.7	0.1				
(Z)-2,5-Dimethyl-3-hexene	C8H16 (20)	10557-44-5					-151.0		-146.0	-5.0				
(E)-2,5-Dimethyl-3-hexene	C8H16 (21)	692-70-6					-159.2		-149.8	-9.4				
(Z)-1-Ethyl-2-methylcyclopentane	C8H16 (22)	930-89-2					-190.8		-195.0	4.2				
(E)-1-Ethyl-2-methylcyclopentane	C8H16 (23)	930-90-5	-156.1	P94	-157.7	1.7	-195.1		-195.0	-0.1				
(Z)-1-Ethyl-3-methylcyclopentane	C8H16 (24)	2613-66-3					-194.4		-195.0	0.6				

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 7

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
(E)-1-Ethyl-3-methylcyclopentane	C8H16 (25)	2613-65-2					-196.0		-195.0	-1.0				
1-Ethyl-1-methylcyclopentane	C8H16 (26)	16747-50-5					-193.8		-198.7	4.9				
(Z)-3-Octene	C8H16	14850-22-7					-132.3	r	-131.0	-1.3				
(E)-3-Octene	C8H16	14919-01-8					-134.3	r	-134.7	0.4				
(Z)-4-Octene	C8H16	7642-15-1					-131.9	r	-131.0	-0.9				
(E)-4-Octene	C8H16	14850-23-8					-135.1	r	-134.7	-0.4				
2-Methyl-1-heptene	C8H16						-139.9	r	-138.1	-1.8				
4-Methyl-1-heptene	C8H16						-127.7	r	-130.1	2.4				
5-Methyl-1-heptene	C8H16						-127.7	r	-130.1	2.4				
6-Methyl-1-heptene	C8H16						-128.6	r	-130.1	1.5				
2-Cyclopropyl-3-methylbutane	C8H16						-61.9	SWS	-111.3	49.4				
2-Cyclopropylpentane	C8H16						-61.9	SWS	-104.6	42.7				
1,2,4-Trimethylcyclopentane	C8H16						-223.0	SWS	-201.7	-21.3				
Octane	C8H18 (1)	111-65-9	-208.6		-209.2	0.6	-250.1		-250.2	0.1				
2-Methylheptane	C8H18 (2)	592-27-8	-215.4		-215.9	0.5	-255.0		-254.6	-0.4				
3-Methylheptane	C8H18 (3)	589-81-1	-212.5		-212.5	0.0	-252.3		-252.3	-0.0				
4-Methylheptane	C8H18 (4)	589-53-7	-212.0		-212.5	0.5	-251.6		-252.3	0.7				
3-Ethylhexane	C8H18 (5)	619-99-8	-210.7		-209.2	-1.5	-250.4		-250.0	-0.4				
2,2-Dimethylhexane	C8H18 (6)	590-73-8	-224.6		-223.8	-0.8	-261.9		-262.8	0.9				
2,3-Dimethylhexane	C8H18 (7)	584-94-1	-213.8		-219.2	5.4	-252.6		-256.7	4.1				
2,4-Dimethylhexane	C8H18 (8)	589-43-5	-219.2		-219.2	0.0	-257.0		-256.7	-0.3				
2,5-Dimethylhexane	C8H18 (9)	592-13-2	-222.5		-222.6	0.1	-260.4		-259.0	-1.4				
3,3-Dimethylhexane	C8H18 (10)	563-16-6	-220.0		-217.1	-2.9	-257.5		-258.2	0.7				
3,4-Dimethylhexane	C8H18 (11)	583-48-2	-212.8		-212.5	-0.3	-251.8		-252.1	0.3				
3-Ethyl-2-methylpentane	C8H18 (12)	609-26-7	-211.0		-215.9	4.9	-249.6		-254.4	4.8				
3-Ethyl-3-methylpentane	C8H18 (13)	1067-08-0	-214.8		-210.5	-4.3	-252.8		-253.6	0.8				
2,2,3-Trimethylpentane	C8H18 (14)	564-02-3	-220.0		-223.8	3.8	-256.9		-262.5	5.6				
2,2,4-Trimethylpentane (Isooctane)	C8H18 (15)	540-84-1	-224.0		-230.5	6.5	-259.2		-267.1	7.9				
2,3,3-Trimethylpentane	C8H18 (16)	560-21-4	-216.3		-220.5	4.2	-253.5		-260.2	6.7				
2,3,4-Trimethylpentane	C8H18 (17)	565-75-3	-217.3		-222.6	5.3	-255.0		-258.8	3.8				
2,2,3,3-Tetramethylbutane	C8H18 (18)	594-82-1	-225.6		-231.8	6.2					-268.9		-256.1	-12.8
1-Phenyl-1-propyne	C9H8	673-32-5	267.8	L	268.2	-0.4								
Indene	C9H8 (1)	95-13-6	163.4		163.6	-0.2	110.6		110.6	-0.0				
1,2-Cyclopentylbenzene (Indane)	C9H10 (1)	496-11-7	60.7		61.1	-0.4	11.5		11.5	0.0				
alpha-Methylstyrene (2-phenylpropene)	C9H10 (2)	98-83-9					70.5		70.3	0.2				
Phenylcyclopropane	C9H10 (3)	873-49-4	150.5		161.9	-11.4	100.3		118.8	-18.5				
2-Propenylbenzene	C9H10 (4)	300-57-2					88.0		94.1	-6.1				
Propylbenzene	C9H12 (1)	103-65-1	7.9		10.0	-2.1	-38.3		-38.9	0.6				
Cumene (isopropylbenzene)	C9H12 (2)	98-82-8	4.0		4.2	-0.2	-41.1		-40.2	-0.9				
m-Ethyltoluene	C9H12 (3)	611-14-3	1.3		-1.7	3.0	-46.4		-50.0	3.6				
o-Ethyltoluene	C9H12 (4)	620-14-4	-1.8		0.8	-2.6	-48.7		-48.4	-0.3				
p-Ethyltoluene	C9H12 (5)	622-96-8	-3.2		-1.7	-1.5	-49.8		-50.0	0.2				

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 8

Compound	Formula (PNK#)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
1,2,3-Trimethylbenzene	C9H12 (6)	526-73-8	-9.5		-10.0	0.5	-58.5		-57.4	-1.1				
1,2,4-Trimethylbenzene	C9H12 (7)	95-63-6	-13.8		-12.6	-1.2	-61.8		-59.1	-2.7				
Mesitylene (1,3,5-Trimethylbenzene)	C9H12 (8)	108-67-8	-15.9		-15.1	-0.8	-63.4		-60.8	-2.6				
(Z)-5-Ethylidene-bicyclo[2.2.1]-2-heptene	C9H12 (9)	28304-66-7	• 145.7		138.9	6.8	102.2		102.1	0.1				
(Z,Z,Z)-1,4,7-Cyclononatriene	C9H12	696-86-6					140.6	l	141.4	-0.8				
(Z)-3a,4,7,7a-Tetrahydro-1H-indene	C9H12	56170-01-5	109.2	s	85.8	23.4	64.3	s	49.0	15.3				
2-Methylene-bicyclo[2.2.2]octane	C9H14 (2)	2972-20-5	-9.2		-7.5	-1.7	-54.4		-52.3	-2.1				
2-Methyl-bicyclo[2.2.2]-2-octene	C9H14 (3)	4893-13-4	-18.6		-19.7	1.1	-61.9		-63.6	1.7				
Bicyclo[3.2.2]-6-nonene	C9H14	7124-86-9	-3.5	t	-3.3	-0.2					-51.5	t	-51.5	-0.0
Bicyclo[3.3.1]-2-nonene	C9H14		-49.1	t	-48.5	-0.6					-97.3	t	-96.7	-0.6
Bicyclo[4.2.1]-3-nonene	C9H14		3.6	t	3.8	-0.2					-46.1	t	-45.6	-0.5
1-Ethyl-4-methyl-1,3-cyclohexadiene	C9H14						-47.7	SWS	-31.4	-16.3				
(Z)-Octahydro-1H-indene	C9H16 (1)	4551-51-3	-127.1		-142.7	15.6	-173.1		-177.4	4.3				
(E)-Octahydro-1H-indene	C9H16 (2)	3296-50-2	-131.5		-147.3	15.8	-176.2		-181.2	5.0				
Cyclohexylcyclopropane	C9H16 (3)	32669-86-6					-314.6		-87.0	-227.6				
(Z)-Bicyclo[6.1.0]nonane	C9H16 (4)	286-60-2	-31.1		-33.1	2.0	-81.0		-79.5	-1.5				
Spiro(4,4)nonane	C9H16 (5)	175-93-9					-143.8		-155.6	11.8				
(E)-(+)-Bicyclo[6.1.0]nonane	C9H16 (6)	39124-79-3	-39.7		-37.7	-2.0	-82.4		-83.3	0.9				
1,4-Dimethyl-bicyclo[2.2.1]heptane	C9H16 (7)	20454-81-3	-128.1		-122.2	-5.9	-167.4		-151.0	-16.4				
(E)-2,3-Dimethyl-bicyclo[2.2.1]heptane	C9H16 (8)	20558-16-1	-107.5		-119.7	12.2	-150.2		-143.5	-6.7				
7,7-Dimethyl-bicyclo[2.2.1]heptane	C9H16 (9)	2034-53-9									-148.2		-144.3	-3.9
2-Ethylbicyclo[2.2.1]heptane	C9H16 (10)	2146-41-0					-140.2		-136.8	-3.4				
Bicyclo[3.3.1]nonane	C9H16 (11)	280-65-9	-127.5		-127.6	0.1					-178.2		-177.8	-0.4
1-Nonyne	C9H16	3452-09-3	62.3	h	61.9	0.3	16.3	h	17.2	-0.9				
2-Nonyne	C9H16	19447-29-1	43.6	h	41.4	2.2	-2.4	h	-7.9	5.6				
3-Nonyne	C9H16	20184-89-8	42.0	h	42.7	-0.7	-4.0	h	-4.6	0.6				
4-Nonyne	C9H16	20184-91-2	42.0	h	42.7	-0.7	-4.0	h	-4.6	0.6				
(Z)-Cyclononene	C9H16	933-21-1					-82.3	q	-81.6	-0.8				
(E)-Cyclononene	C9H16						-70.3	q	-69.9	-0.5				
2-Cyclopropyl-1-hexene	C9H16						46.9	SWS	-12.1	59.0				
2-Cyclopropyl-2-hexene	C9H16						-15.9	SWS	-23.4	7.5				
1-Isopropylcyclohexene	C9H16						-213.0	SWS	-139.7	-73.2				
Propylcyclohexane	C9H18 (1)	1678-92-8	-192.5		-195.4	2.9	-237.4		-239.3	1.9				
(1a,3a,5a)-1,3,5-Trimethylcyclohexane	C9H18 (2)	1795-27-3	-212.1		-215.5	3.4								
Cyclononane	C9H18 (3)	293-55-0	-132.8		-132.6	-0.2	-181.2		-180.7	-0.5				
1-Ethyl-1-methylcyclohexane	C9H18 (4)	4926-90-3					-240.2		-249.8	9.6				
(Z)-1-Ethyl-2-methylcyclohexane	C9H18 (5)	4923-77-7					-236.2		-239.1	2.9				
(E)-1-Ethyl-2-methylcyclohexane	C9H18 (6)	4923-78-8					-240.2		-243.7	3.5				
(Z)-1-Ethyl-3-methylcyclohexane	C9H18 (7)	19489-10-2					-247.1		-246.0	-1.1				
(Z)-1-Ethyl-4-methylcyclohexane	C9H18 (8)	4926-78-7					-238.9		-241.4	2.5				
(E)-1-Ethyl-4-methylcyclohexane	C9H18 (9)	6236-88-0					-246.4		-246.0	-0.4				
1-Nonene	C9H18	124-11-8					-149.0	DH	-149.0	-0.1				

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 9

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
Butylcyclopentane	C9H18		-214.3	SWS	-195.4	-18.9								
Cyclopropylhexane	C9H18		-69.5	SWS	-82.4	13.0								
Methyl-1-propylcyclopentane	C9H18		-249.4	SWS	-206.7	-42.7								
1,1,3-Trimethylcyclohexane	C9H18		-277.4	SWS	-216.7	-60.7								
1,2,3-Trimethylcyclohexane	C9H18		-272.4	SWS	-215.5	-56.9								
Ethylcycloheptane	C9H18		-226.8	SWS	-160.2	-66.5								
Nonane	C9H20 (1)	111-84-2	-228.2		-230.1	1.9	-274.7		-275.7	1.0				
3,3-Diethylpentane	C9H20 (2)	1067-20-5	-232.3		-224.7	-7.6	-275.4		-274.5	-0.9				
2,2,3,3-Tetramethylpentane	C9H20 (3)	7154-79-2	-237.1		-246.0	8.9	-278.3		-291.6	13.3				
2,2,3,4-Tetramethylpentane	C9H20 (4)	1186-53-4	-236.9		-244.8	7.9	-277.7		-283.8	6.1				
2,2,4,4-Tetramethylpentane	C9H20 (5)	1070-87-7	-241.6		-246.0	4.4	-280.0		-283.5	3.5				
2,3,3,4-Tetramethylpentane	C9H20 (6)	16747-38-9	-236.1		-244.8	8.7	-277.9		-287.9	10.0				
3,3,4-Trimethylhexane	C9H20 (7)	16747-31-2					-277.5		-288.1	10.6				
2,2,3-Trimethylhexane	C9H20 (8)	16757-25-4					-282.7		-288.1	5.4				
2,2,5-Trimethylhexane	C9H20 (9)	3522-94-9	-253.1	P94	-251.5	-1.7	-293.3		-292.7	-0.6				
2,2,4-Trimethylhexane	C9H20 (10)	16747-26-5					-282.8		-292.7	9.9				
2,2-Dimethylheptane	C9H20 (11)	1071-26-7					-288.2		-288.3	0.1				
2,4,4-Trimethylhexane	C9H20 (12)	16747-30-1					-280.2		-292.7	12.5				
2,3,5-Trimethylhexane	C9H20 (13)	1069-53-0	-242.7	P94	-243.5	0.8	-284.0		-284.3	0.3				
2,3,3-Trimethylhexane	C9H20 (14)	16747-28-7					-281.1		-283.5	2.4				
3-Ethyl-2,2-dimethylpentane	C9H20 (15)	16747-32-3					-272.7		-283.5	10.8				
3-Ethyl-2,4-dimethylpentane	C9H20 (16)	1068-87-7					-269.7		-272.8	3.1				
Azulene	C10H8 (1)	275-51-4	289.1		289.5	-0.4					212.3		211.7	0.6
Naphthalene	C10H8 (2)	91-20-3	150.3		149.8	0.5					77.9		85.4	-7.5
1-Phenyl-1-butyne	C10H10	622-76-4	249.4	u	248.5	0.8								
1,2-Dihydronaphthalene	C10H10 (1)	447-53-0	117.2	L	117.6	-0.4	71.5		71.7	-0.2				
1,4-Dihydronaphthalene	C10H10 (2)	612-17-9					84.2		51.6	32.6				
2,7-Dimethyl-oct-1,7-dien-3,5-diyne	C10H10		494.1	c	493.7	0.4								
Triquinacine	C10H10	6053-74-3	223.8	v	211.3	12.6								
4-Phenyl-1-butyne	C10H10						245.2	SWS	228.4	16.7				
Tetralin (1,2,3,4-Tetrahydronaphthalene)	C10H12 (1)	119-64-2	26.0		25.9	0.1	-29.2		-29.1	-0.1				
3a,4,7,7a[all alpha]-Tetrahydro-4,7-methano... -1H-indene (Tetracyclo[5.2.1.0^2,6]decane)	C10H12 (2)	1755-01-7									116.7		116.7	-0.0
3a,4,7,7a-Tetrahydro-4,7-methano-1H-indene	C10H12 (3)	77-73-6	196.1	w	196.2	-0.1								
3-Phenyl-1-butene	C10H12 (4)	934-10-1					56.1		56.5	-0.4				
1-Phenyl-1-butene	C10H12						-7.1	SWS	38.9	-46.0				
1-Phenyl-2-butene	C10H12						56.1	SWS	57.3	-1.3				
2-Phenyl-2-butene	C10H12										39.3	SWS	17.6	21.8
4-Phenyl-1-butene	C10H12						30.1	SWS	62.3	-32.2				
Tetracyclo[5.2.1.0^2,6.0^3,5]-8-decene	C10H12	6574-77-2					252.7	g	252.7					
Dihydrotriquinacine	C10H12	31678-74-7	127.6	v	166.1	-38.5								
Butylbenzene (1-Phenylbutane)	C10H14 (1)	104-51-8	-13.1		-10.9	-2.2	-63.2		-64.4	1.2				

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 10

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
Isobutylbenzene	C10H14 (2)	538-93-2	-21.5		-20.9	-0.6	-69.8		-71.1	1.3				
sec-Butylbenzene (2-Phenylbutane)	C10H14 (3)	135-98-8	-17.4		-16.7	-0.7	-66.4		-65.7	-0.7				
tert-Butylbenzene	C10H14 (4)	98-06-6	-22.6		-21.3	-1.3	-70.7		-70.3	-0.4				
1,2,3,4-Tetramethylbenzene	C10H14 (5)	488-23-3					-90.2		-92.4	2.2				
1,2,3,5-Tetramethylbenzene	C10H14 (6)	527-53-7					-96.4		-94.1	-2.3				
1,2,4,5-Tetramethylbenzene (Durene)	C10H14 (7)	95-93-2									-119.9		-107.9	-12.0
3a,4,5,6,7,7a-Hexahydro-4,7-methanoindene	C10H14 (8)	4488-57-7									-23.9		-7.5	-16.4
1-Methyl-2-propylbenzene	C10H14 (9)	1074-17-5					-72.5		-73.9	1.4				
1-Methyl-3-propylbenzene	C10H14 (10)	1074-43-7					-76.2		-75.6	-0.6				
1-Methyl-4-propylbenzene	C10H14 (11)	1074-55-1					-75.1		-75.6	0.5				
1-Isopropyl-2-methylbenzene (o-Cymene)	C10H14 (12)	527-84-4					-73.3		-75.1	1.8				
1-Isopropyl-3-methylbenzene (m-Cymene)	C10H14 (13)	535-77-3					-78.6		-76.8	-1.8				
1-Isopropyl-4-methylbenzene (p-Cymene)	C10H14 (14)	99-87-6					-78.0		-76.8	-1.2				
1,2-Diethylbenzene	C10H14 (15)	135-01-3					-68.5		-74.3	5.8				
1,3-Diethylbenzene	C10H14 (16)	141-93-5					-73.5		-76.0	2.5				
1,4-Diethylbenzene	C10H14 (17)	105-05-5					-72.8		-76.0	3.2				
1-Ethyl-2,3-dimethylbenzene	C10H14 (18)	933-98-2					-80.5		-83.3	2.8				
4-Ethyl-1,2-dimethylbenzene	C10H14 (19)	934-80-5					-86.0		-85.0	-1.0				
2-Ethyl-1,3-dimethylbenzene	C10H14 (20)	2870-04-4					-80.1		-83.3	3.2				
1-Ethyl-2,4-dimethylbenzene	C10H14 (21)	874-41-9					-84.1		-85.0	0.9				
1-Ethyl-3,5-dimethylbenzene	C10H14 (22)	934-74-7					-87.8		-86.7	-1.1				
2-Ethyl-1,4-dimethylbenzene	C10H14 (23)	1758-88-9					-84.8		-85.0	0.2				
Tetrahydrotriquinacine	C10H14		12.6	v	-16.7	29.3								
(Z)-3-Decen-1-yne	C10H16 (1)	61827-88-1	145.9	b	146.0	-0.1	99.2		99.2	0.0				
(E)-3-Decen-1-yne	C10H16 (2)	2807-10-5	148.7	b	149.0	-0.3	100.5		101.7	-1.2				
2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene (alpha-Pinene)	C10H16 (3)	80-56-8	28.3		33.5	-5.2	-16.4		-10.0	-6.4				
6,6-Dimethyl-2-methylene-bicyclo[3.1.1]heptane (beta-Pinene)	C10H16 (4)	127-91-3	38.7		33.9	4.8	-7.7		-15.1	7.4				
(+)-Limonene	C10H16 (5)	7705-14-8	-6.4		-5.0	-1.4	-54.5		-52.3	-2.2				
(+-)-Limonene	C10H16 (6)	7705-14-8	-2.6		-5.0	2.4	-50.8		-52.3	1.5				
2,6-Dimethyl-2,4,6-octatriene ((Z)-Allocimene)	C10H16 (7)	673-84-7					-24.0		-21.3	-2.7				
7-Methyl-3-methylene-1,6-octadiene (Myrcene)	C10H16 (8)	123-35-3					14.5		25.1	-10.6				
5-Isopropyl-2-methyl-1,3-cyclohexadiene	C10H16 (9)	99-83-2	-9.3		-8.8	-0.5	-60.0	x	-53.6	-6.4				
1-Isopropyl-4-methyl-1,3-cyclohexadiene	C10H16 (10)	99-86-5	-20.6		-16.7	-3.9								
Octahydro-4,7-methano-indene	C10H16 (11)	6004-38-2	-60.0		-59.8	-0.2	-110.0		-110.0	0.0	-112.9		-129.7	16.8
Adamantane	C10H16 (12)	281-23-2	-134.6		-134.7	0.1					-194.1		-193.7	-0.4
Perhydroquinacene	C10H16 (14)		-102.3		-102.5	0.2					-159.0		-159.0	-0.0
2,2-Dimethyl-3-methylene-bicyclo[2.2.1]heptane (Camphene)	C10H16 (15)	79-92-5	-28.6		-20.5	-8.1					-75.4		-74.9	-0.5
Bicyclopentyl	C10H18 (1)	1636-39-1					-178.9		-177.4	-1.5				
(Z)-Decalin (cis-Decahydronaphthalene)	C10H18 (2)	493-01-6	-169.2		-171.5	2.3	-219.4		-221.5	2.1				

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 11

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
(E)-Decalin (trans-Decahydronaphthalene)	C10H18 (3)	493-02-7	-182.1		-181.6	-0.5	-230.6		-228.4	-2.2				
Perhydroazulene (Bicyclo[5.3.0]decane)	C10H18 (4)	5661-80-3	-130.8		-131.0	0.2	-183.7		-183.7	-0.0				
Spiro(4,5)decane	C10H18 (5)	176-63-6	-145.1		-156.1	11.0	-200.0		-206.7	6.7				
Bicyclo[3.3.2]decane	C10H18 (6)	283-50-1	-106.1		-106.3	0.2					-164.2		-164.0	-0.2
(Z)-3,7,7-Trimethyl-bicyclo[4.1.0]heptane	C10H18 (7)	18968-23-5	-69.8		-65.7	-4.1	-115.9		-118.4	2.5				
(E)-3,7,7-Trimethyl-bicyclo[4.1.0]heptane	C10H18 (8)	18968-24-6	-72.1		-65.7	-6.4	-118.5		-118.4	-0.1				
1-Decyne	C10H18	764-93-2	41.9	h	41.0	0.9	-9.5	h	-8.4	-1.1				
2-Decyne	C10H18	2384-70-5	23.6	h	20.5	3.1	-27.8	h	-33.5	5.6				
3-Decyne	C10H18	2384-85-2	21.8	h	21.8	0.1	-29.5	h	-30.1	0.6				
4-Decyne	C10H18	2384-86-3	19.9	h	21.8	-1.9	-31.5	h	-30.1	-1.4				
5-Decyne	C10H18	1942-46-7	18.7	h	21.8	-3.1	-32.7	h	-30.1	-2.6				
(Z)-Cyclodecene	C10H18	935-31-9					-120.2	q	-119.7	-0.5				
(E)-Cyclodecene	C10H18	2198-20-1					-106.2	q	-105.4	-0.8				
1-Decene	C10H20 (1)	872-05-9	-123.4		-125.1	1.7	-173.8		-174.5	0.7				
(Z)-2,2,5,5-tetramethyl-3-hexene	C10H20 (2)	692-47-7					-163.6		-164.4	0.8				
(E)-2,2,5,5-tetramethyl-3-hexene	C10H20 (3)	692-48-8	-165.5		-164.8	-0.7	-207.5		-207.5	0.0				
Butylcyclohexane	C10H20 (4)	1678-93-9	-213.3		-216.3	3.0	-263.1		-264.8	1.7				
1-Methyl-4-(1-methylethyl)-cyclohexane	C10H20 (5)	99-82-1	-230.7		-233.0	2.3								
Cyclodecane	C10H20 (6)	293-96-9	-154.3		-154.4	0.1	-206.7		-206.3	-0.4				
Decane	C10H22 (1)	124-18-5	-249.5		-251.0	1.5	-300.9		-301.2	0.3				
2-Methylnorane	C10H22 (2)	871-83-0	-259.9		-257.7	-2.2	-309.8		-305.6	-4.2				
5-Methylnorane	C10H22 (3)	15869-85-9	-258.6		-254.4	-4.2	-307.9		-303.3	-4.6				
2,3-Cyclopropylnaphthalene	C11H8	286-85-1	435.1	L	437.6	-2.5								
1-Methylnaphthalene	C11H10 (1)	90-12-0	113.0	L	117.2	-4.2	56.3		56.6	-0.3				
2-Methylnaphthalene	C11H10 (2)	91-57-6	106.7		117.2	-10.5					44.9		49.0	-4.1
Bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene	C11H10 (3)	2443-46-1	315.0		315.9	-0.9	254.2		254.0	0.2				
1-Methyltetralin	C11H14 (1)	1559-81-5					-67.7		-58.0	-9.7				
1,1-Dimethylindane	C11H14 (2)	4912-92-9	-1.6		8.8	-10.4	-53.6		-45.4	-8.2				
4,6-Dimethylindane	C11H14 (3)	1685-82-1	-5.8		-4.2	-1.6	-63.7		-61.8	-1.9				
4,7-Dimethylindane	C11H14 (4)	6682-71-9	-7.4		-4.2	-3.2	-65.7		-61.8	-3.9				
Pentamethylbenzene	C11H16 (1)	700-12-9	-74.5	DH	-70.3	-4.2					-133.6		-134.3	0.7
Pentylbenzene	C11H16 (2)	538-68-1	-34.3	DH	-31.8	-2.5	-89.5		-90.0	0.5				
1-Methyladamantane	C11H18 (1)	768-91-2	-171.6		-166.9	-4.7					-239.3		-225.5	-13.8
2-Methyladamantane	C11H18 (2)	700-56-1	-151.7		-162.3	10.6					-219.6		-221.8	2.2
Dicyclopentylmethane	C11H20 (1)	2619-34-3					-205.1		-202.9	-2.2				
Cyclopentylcyclohexane	C11H20 (2)	1606-08-2					-230.2		-228.4	-1.8				
(E)-2-Methyl-decahydronaphthalene	C11H20 (3)	4683-94-7					-264.9		-260.7	-4.2				
(Z)-4a-Methyl-decahydronaphthalene	C11H20 (4)	2547-26-4					-243.8		-252.9	9.1				
(E)-4a-Methyl-decahydronaphthalene	C11H20 (5)	2547-27-5					-249.7		-255.2	5.5				
Spiro(5,5)undecane	C11H20 (6)	180-43-8	-188.3		-177.0	-11.3	-244.5		-239.3	-5.2				
Bicyclo[3.3.3]undecane	C11H20 (7)	29415-95-0	-89.0		-89.1	0.1					-152.5		-152.3	-0.2
1,1-Dimethyl-2-hexylcyclopropane	C11H22 (1)	41845-49-2					-193.0		-191.6	-1.4				

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 12

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
Cycloundecane	C11H22 (2)	294-41-7	-179.4		-179.5	0.1	-235.5		-235.1	-0.4				
Undecane	C11H24 (1)	1120-21-4	-270.9		-272.0	1.1	-327.2		-326.8	-0.4				
2,2,5,5-Tetramethylheptane	C11H24 (2)	61868-47-1	-302.4		-294.6	-7.8	-351.2		-347.3	-3.9				
3,3,5,5-Tetramethylheptane	C11H24 (3)	61868-61-9	-276.7		-274.5	-2.2	-325.7		-325.3	-0.4				
2,2,4,4,5,-Pentamethylhexane	C11H24 (4)	60302-23-0	-281.0		-284.5	3.5	-329.0		-332.0	3.0				
Biphenylene	C12H8 (1)	259-79-0	417.9		417.6	0.3					334.0		334.3	-0.3
Acenaphthylene	C12H8 (2)	208-96-8	259.7		254.8	4.9					186.7		174.5	12.2
Biphenyl	C12H10 (1)	92-52-4	181.4		181.6	-0.2	116.0		123.8	-7.8	99.4		99.6	-0.2
1,8-Cyclopentylnaphthalene (Acenaphthene)	C12H10 (2)	83-32-9	156.0		156.9	-0.9					70.3		70.7	-0.4
1,8-Dimethylnaphthalene	C12H12 (1)	569-41-5	108.7		106.7	2.0	41.8		47.1	-5.3	25.9		33.5	-7.6
2,3-Dimethylnaphthalene	C12H12 (2)	581-40-8									-2.3		12.6	-14.9
2,6-Dimethylnaphthalene	C12H12 (3)	581-42-0									-5.7		12.6	-18.3
2,7-Dimethylnaphthalene	C12H12 (4)	582-16-1									-5.4		12.6	-18.0
1-Phenylcyclohexene	C12H14 (2)	771-98-2					-16.8	*	25.1	-41.9				
Dicyclohexadiene	C12H16 (1)						26.2		17.6	8.6				
(Z)-1-Phenyl-3,3-dimethyl-1-butene	C12H16 (2)	3740-05-4	66.9	L	57.7	9.2	10.0	y	-7.9	17.9				
(E)-1-Phenyl-3,3-dimethyl-1-butene	C12H16 (3)	3846-66-0	33.5	L	39.3	-5.9	-22.6		-23.0	0.4				
Cyclohexylbenzene	C12H16 (4)	827-52-1	-16.7		-13.8	-2.9	-76.6		-73.6	-3.0				
3,9-Dodecadiyne	C12H18 (1)	61827-89-2	251.6	b	252.7	-1.1	197.8		190.0	7.8				
5,7-Dodecadiyne	C12H18 (2)	1120-29-2	235.6	b	233.5	2.2	181.5		180.7	0.8				
Hexamethylbenzene	C12H18 (3)	87-85-4	-86.8		-97.9	11.1					-161.5		-165.7	4.2
3,3,6,6-Tetramethyl-octa-1,7-diyne	C12H18 (4)	64020-56-0	257.2	b	271.1	-13.9	211.1		210.9	0.2				
(E,E,Z)-1,5,9-Cyclododecatriene	C12H18 (5)	706-31-0	97.1		97.9	-0.8	29.9		31.4	-1.5				
(E,E,E)-1,5,9-Cyclododecatriene	C12H18 (6)	676-22-2	101.3		102.5	-1.2					26.6		27.6	-1.0
2,2,7,7-Tetramethylocta-3,5-diyne	C12H18 (7)	6130-98-9									156.1		157.3	-1.2
2,2-Dimethyladamantane	C12H20 (2)	19740-34-2	-182.7		-184.5	1.8					-256.3		-248.5	-7.8
1,3-Dimethyladamantane	C12H20 (3)	702-79-4	-218.7		-199.2	-19.5					-286.4		-257.3	-29.1
Bicyclohexyl	C12H22 (1)	92-51-3	-215.7		-223.4	7.7	-273.7		-279.5	5.8				
Cyclopentylcycloheptane	C12H22 (2)	43247-48-8					-226.3		-228.9	2.6				
Spiro(5,6)dodecane	C12H22 (3)	181-15-7					-253.0		-239.7	-13.3				
Cyclododecane	C12H24 (1)	2199-46-6	-230.2		-230.1	-0.1					-306.6		-305.4	-1.2
1-Dodecene	C12H24 (2)	643-58-3	-165.4		-166.9	1.5	-226.2	i	-225.5	-0.7				
Dodecane	C12H26 (1)	643-93-6	-289.7		-292.9	3.2	-350.9		-352.3	1.4				
3,3,6,6-Tetramethyloctane	C12H26 (2)	644-08-6	-318.2		-308.8	-9.4	-372.8		-368.2	-4.6				
2-Methyl-1,1'-biphenyl	C13H12 (1)	643-58-3	171.5	L	151.5	20.1	108.2		88.9	19.3				
3-Methyl-1,1'-biphenyl	C13H12 (2)	643-93-6					85.6		87.2	-1.6				
4-Methyl-1,1'-biphenyl	C13H12 (3)	644-08-6									55.4		63.2	-7.8
Diphenylmethane	C13H12 (4)	101-81-5	157.2		157.7	-0.5	89.7		100.4	-10.7	71.5		61.9	9.6
1,1,4,6-Tetramethylindane	C13H18 (1)	941-60-6	-70.5		-56.5	-14.0	-131.8		-118.7	-13.1				
1,1,4,7-Tetramethylindane	C13H18 (2)	1078-04-2	-62.5		-56.5	-6.0	-123.9		-118.7	-5.2				
2,5,8-Trimethyldecalin	C13H18 (3)	30316-17-7					-135.6		-136.7	1.1				
1,3,5-Trimethyladamantane	C13H22 (1)	707-35-7	-254.5		-231.4	-23.1					-332.3		-289.1	-43.2

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 13

Compound	Formula (PNK#)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
Heptylcyclohexane	C13H26 (1)	5617-41-4	-289.2		-279.1	-10.1	-353.0		-341.4	-11.6				
Cyclotridecane	C13H26 (2)	295-02-3	-246.4		-246.4	0.0	-309.7		-309.2	-0.5				
4,4,6,6-Tetramethylnonane	C13H28 (1)	74286-93-4	-313.2		-323.0	9.8	-371.0		-381.0	10.0				
3,5-Diethyl-3,5-dimethylheptane	C13H28 (2)	74286-94-5	-301.3		-302.9	1.6	-360.5		-367.2	6.7				
Diphenylacetylene (Tolane)	C14H10 (1)	501-65-5	401.7	L	391.6	10.0					312.4		305.4	7.0
Anthracene	C14H10 (2)	120-12-7	230.9		216.7	14.2					129.2		133.1	-3.9
Phenanthrene	C14H10 (3)	85-01-8	201.3	d	214.2	-13.0					109.6	d	122.2	-12.6
9,10-Dihydroanthracene	C14H12 (1)	613-31-0	159.7		159.0	0.7					66.4		63.2	3.2
1,1-Diphenylethylene	C14H12 (2)	530-48-3	245.6		243.9	1.7	172.4		172.8	-0.4				
(Z)-Stilbene	C14H12 (3)	645-49-8	252.3		248.1	4.2	183.3		165.3	18.0				
(E)-Stilbene	C14H12 (4)	103-30-0	236.1		243.5	-7.4					136.9		136.4	0.5
9,10-Dihydrophenanthrene	C14H12 (5)	776-35-2					78.7	P94	78.6	0.1				
3,3'-Dimethylbiphenyl	C14H14 (1)	612-75-9					20.0		50.5	-30.5				
4,4'-Dimethylbiphenyl	C14H14 (2)	613-33-2									14.1		26.8	-12.7
1,1-Diphenylethane	C14H14 (3)	612-00-0					48.7		46.4	2.3				
Bibenzyl (1,2-Diphenylethane)	C14H14 (4)	103-29-7	142.9		145.6	-2.7					51.5		32.6	18.9
4-Methyldiphenylmethane	C14H14 (5)	620-83-7					61.5		63.8	-2.3				
1,4,5,8-Tetramethylnaphthalene	C14H16 (1)	2717-39-7	81.6		63.6	18.0	5.7		1.0	4.7	-18.2		-18.4	0.2
2-tert-Butylnaphthalene	C14H16 (3)	2876-35-9					-26.3		-26.3	-0.0				
Octhracene (octahydroanthracene)	C14H18 (1)	1079-71-6	-37.2		-37.2	0.0	-101.6		-101.6	-0.0	-119.5	z	-119.7	0.2
1,8-Cyclotetradecadiyne	C14H20 (1)	1540-80-3	313.8		315.1	-1.3					147.8		147.3	0.5
Diamantane (Diadamantane; Congressane)	C14H20 (2)	2292-79-7	-145.9		-138.9	-7.0	-211.7		-211.7	0.0	-241.8		-230.1	-11.7
2,3-Dihydro-1,1,4,6,7-pentamethyl-1H-indene	C14H20 (3)	6682-67-3									-175.1		-174.9	-0.2
Para-di-tert-butylbenzene	C14H22	1012-72-2	-121.3	L	-125.5	4.2	-189.1	ab	-189.8	0.7				
Meta-di-tert-butylbenzene	C14H22	1014-60-4	-125.5	L	-125.5		-187.4	ab	-189.8	2.3				
(E)-anti-(E)-Tetradecahydroanthracene	C14H24 (1)	28071-99-0	-220.6		-220.5	-0.1					-293.3		-330.5	37.2
(E)-syn-(E)-Tetradecahydroanthracene	C14H24 (2)	28071-99-0	-243.2		-233.9	-9.3					-330.6		-356.5	25.9
1,3,5,7-Tetramethyladamantane	C14H24 (3)	1687-36-1	-283.4		-262.3	-21.1					-365.8		-318.8	-47.0
1,2-Dicyclohexylethane	C14H26 (1)	3321-50-4					-382.0		-325.9	-56.1				
Bicycloheptyl	C14H26 (2)	23183-11-1					-285.0		-273.4	-11.6				
Cyclotetradecane	C14H28 (1)	295-17-0	-239.2		-268.6	29.4					-374.0		-374.0	0.0
(Z)-1,4-Di-tert-butylcyclohexane	C14H28 (2)	4789-34-8					-365.3		-367.6	2.3	-374.1		-374.0	-0.1
(E)-1,4-Di-tert-butylcyclohexane	C14H28 (3)	4789-35-9					-384.5		-384.9	0.4	-401.8		-400.0	-1.8
1,1,4,4-Tetramethylcyclodecane	C14H28 (4)	15841-11-9					-338.0		-342.7	4.7				
1,1,5,5-Tetramethylcyclodecane	C14H28 (5)	16723-89-0					-328.6		-342.7	14.1				
4-Methylphenanthrene	C15H12 (1)	832-64-4									102.5	P94	96.7	5.9
1,1-Diphenylcyclopropane	C15H14 (1)	3282-18-6					185.5		162.3	23.2				
(Z)-1,2-diphenylcyclopropane	C15H14 (2)	1138-48-3	251.0	L	245.2	5.9	178.8		161.5	17.3				
(E)-1,2-diphenylcyclopropane	C15H14 (3)	1138-47-2	238.5	L	240.6	-2.1	166.2		157.7	8.5				
2,5-Dimethyldiphenylmethane	C15H16 (1)						24.7		28.8	-4.1				
7-Isopropyl-1,4-dimethylazulene (Guaiazulene)	C15H18 (1)	489-84-9									61.1		61.5	-0.4
4-Methyldiadamantane	C15H22 (1)	30545-18-9	-182.1		-171.1	-11.0					-261.5		-261.9	0.4

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 14

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
3-Methyldadamantane	C15H22 (2)	36375-86-2	-157.3		-171.1	13.8					-260.4		-261.9	1.5
1-Methyldadamantane	C15H22 (3)	26460-76-4	-166.7		-171.1	4.4					-247.4		-261.9	14.5
6-tert-Butyl-1,1-dimethylindane	C15H22 (4)						-174.3		-164.9	-9.4				
Decylcyclopentane	C15H30 (1)	1795-21-7					-367.3		-366.9	-0.4				
Cyclopentadecane	C15H30 (2)	295-48-7	-301.4		-301.2	-0.2					-376.1		-376.6	0.5
5,5,7,7-Tetramethylundecane	C15H32 (1)	74286-95-6	-366.6		-371.5	4.9	-433.5		-436.6	3.1				
4,6-Diethyl-4,6-dimethylnonane	C15H32 (2)	74286-96-7	-347.1		-344.8	-2.3	-414.7		-418.2	3.5				
1,4-Diphenyl-1,3-butadiyne	C16H10 (1)	886-66-8									518.4		512.1	6.3
Fluoranthene (1,2-Benzacenaphthene)	C16H10 (2)	206-44-0	289.0		289.5	-0.5					189.9		190.4	-0.5
Pyrene	C16H10 (3)	129-00-0	225.7		236.8	-11.1					125.5		140.6	-15.1
Bis(2-methylphenyl)acetylene	C16H14 (1)	5294-03-1									234.8		237.7	-2.9
Bis(4-methylphenyl)acetylene	C16H14 (2)	2789-88-0									225.8		232.6	-6.8
(Z,Z)-1,4-Diphenyl-1,3-butadiene	C16H14 (3)	5807-76-1									198.8		179.9	18.9
1,4-Diphenyl-1,3-butadiene	C16H14 (4)	538-81-8									178.8		179.9	-1.1
2,7-Dimethylphenanthrene	C16H14 (5)	1576-69-8	143.1		149.0	-5.9					36.4		49.4	-13.0
4,5-Dimethylphenanthrene	C16H14 (6)	3674-69-9	193.6		192.9	0.7					89.0		91.2	-2.2
9,10-Dimethylphenanthrene	C16H14 (7)	604-83-1	167.1		151.5	15.6					47.6		51.9	-4.3
1,1-Bis(2-methylphenyl)ethylene	C16H16 (1)	2919-19-9									89.0		108.8	-19.8
(Z)-1,2-Bis(2-methylphenyl)ethylene	C16H16 (2)	10311-74-7									85.9		72.8	13.1
(E)-1,2-Bis(2-methylphenyl)ethylene	C16H16 (3)	36888-18-3									74.9		68.6	6.3
1,1-Bis(4-methylphenyl)ethylene	C16H16 (4)	2919-20-2									85.9		103.8	-17.9
(Z)-1,2-Bis(4-methylphenyl)ethylene	C16H16 (5)	2510-76-1									97.9		67.8	30.1
(E)-1,2-Bis(4-methylphenyl)ethylene	C16H16 (6)	18869-29-9									57.9		63.6	-5.7
1,3,5,7,9,11,13,15-Cyclohexadecaoctaene	C16H16 (10)	3332-38-5									547.5		548.9	-1.4
1,1-Bis(2-methylphenyl)ethane	C16H18 (1)	33268-48-3					-26.1		-23.5	-2.6				
1,2-Bis(2-methylphenyl)ethane	C16H18 (2)	952-80-7									-40.0		-35.1	-4.9
1,1-Bis(4-methylphenyl)ethane	C16H18 (3)	530-45-0					-33.2		-26.9	-6.3				
1,2-Bis(4-methylphenyl)ethane	C16H18 (4)	538-39-6									-42.1		-40.2	-1.9
1,4-Diphenylbutane	C16H18 (5)	1083-56-3									-9.9		-25.9	16.0
Decylbenzene	C16H26 (1)	104-72-3	-138.6		-136.4	-2.2	-218.3		-217.6	-0.7				
1-Hexadecene	C16H32 (1)	629-73-2	-248.5		-250.6	2.1	-328.7		-327.6	-1.1				
Decylcyclohexane	C16H32 (2)	1795-16-0	-339.5		-341.8	2.3	-418.2		-418.0	-0.2				
Cyclohexadecane	C16H32 (3)	295-65-8	-321.7		-322.2	0.5					-403.4		-403.3	-0.1
Hexadecane	C16H34 (1)	544-76-3	-374.8		-376.6	1.8	-456.1		-454.4	-1.7				
Cycloheptadecane	C17H34 (1)	295-97-6	-364.3		-364.4	0.1					-430.4		-431.0	0.6
Triphenylene	C18H12 (1)	217-59-4	274.2		276.1	-1.9					151.8		148.1	3.7
Chrysene	C18H12 (2)	218-01-9	269.8		278.7	-8.9					145.3		159.0	-13.7
Benzo[c]phenanthrene	C18H12 (3)	195-19-7	291.2		279.9	11.3					184.9		164.4	20.5
Benz[a]arthracene	C18H12 (4)	56-55-3	293.0		281.2	11.8					170.8		169.9	0.9
Naphthacene	C18H12 (5)	92-24-0	283.3	z	283.7	-0.4					158.8		180.7	-21.9
5,12-Dihydronaphthacene	C18H14 (1)	959-02-4	222.3		225.9	-3.6					106.4		110.9	-4.5
6,6-Diphenylfulvene	C18H14 (2)	2175-90-8	402.0		417.1	-15.1					297.4		297.1	0.3

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 15

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
1,3,5,7,9,11,13,15,17-Cyclooctadecanonaene	C18H18 (1)	2040-73-5									401.7	w	401.7	-0.0
3,4,5,6-Tetramethylphenanthrene	C18H18 (2)	7343-06-8	156.9		132.6	24.3					23.4		23.4	-0.0
2,4,5,7-Tetramethylphenanthrene	C18H18 (3)	7396-38-5	126.4		127.6	-1.2					12.2		18.4	-6.2
Dodecahydrotriphenylene	C18H24 (1)	1610-39-5									-193.9	aa	-193.7	-0.2
1,2,4-Tri-tert-butylbenzene	C18H30 (1)	1459-11-6	-142.3	L	-142.7	0.4					-251.6		-248.5	-3.1
1,3,5-Tri-tert-butylbenzene	C18H30 (2)	1460-02-2	-242.7	L	-229.7	-13.0	-306.7	ab	-309.3	2.6	-321.9		-320.1	-1.8
Dodecylcyclohexane	C18H36 (1)	1795-17-1	-378.7		-383.7	5.0	-467.6		-469.0	1.4				
Octadecane	C18H38 (1)	593-45-3	-414.6		-418.4	3.8					-567.4		-553.1	-14.3
Triphenylmethane	C19H16 (1)	519-73-3	271.2		272.0	-0.8					171.2		171.5	-0.3
Bis(2,4,5-trimethylphenyl)-methane	C19H24 (1)	4957-16-8									-154.4		-146.4	-8.0
Perylene	C20H12 (1)	198-55-0	309.6	L	298.7	10.9					182.8		166.5	16.3
9,10-Dihydro-9,10[1'.2']-benzenoarthracene	C20H14 (1)	477-75-8	321.7		321.7	-0.0					217.1		217.1	-0.0
Triphenylethylene	C20H16 (1)	58-72-0									233.4		223.8	9.6
5,8-Dimethylbenzo[c]phenanthrene	C20H16 (2)										108.2		107.9	0.3
1,12-Dimethylbenzo[c]phenanthrene	C20H16 (3)	4076-43-1									154.5		149.8	4.7
3,9-Dimethylbenz[a]-anthracene	C20H16 (4)	316-51-8	188.7		215.9	-27.2					76.2		97.1	-20.9
1,12-Dimethylbenz[a]-anthracene	C20H16 (5)	313-74-6	251.5		259.8	-8.3					139.0		138.9	0.1
7,12-Dimethylbenz[a]-anthracene	C20H16 (6)	57-97-6	277.7		237.9	39.8					143.8		118.0	25.8
5,6-Dimethylchrysene	C20H16 (7)	3697-27-6	262.4		240.4	22.0					132.5		112.1	20.4
1,1,1-Triphenylethane	C20H18 (1)	5271-39-6									157.2		213.8	-56.6
1,1,2-Triphenylethane	C20H18 (2)	1520-42-9									130.2		126.8	3.4
1-Naphthyl-2-naphthylmethane	C21H16 (1)	611-48-3									162.0		157.3	4.7
1',2',3',4'-Tetrahydro-1',2'-binaphthylmethane	C21H20 (1)	56818-06-5									44.1		11.3	32.8
1,2,4,5-Tetra-tert-butylbenzene	C22H38 (1)	796-97-4									-297.9		-296.2	-1.7
Tris(2-methylphenyl)-ethylene	C23H22 (1)										125.2		122.2	3.0
Tris(4-methylphenyl)-ethylene	C23H22 (2)	6629-83-9									121.2		114.6	6.6
1,1,2-Tris(2-methylphenyl)-ethane	C23H24 (1)										24.4		25.1	-0.7
1,1,2-Tris(4-methylphenyl)-ethane	C23H24 (2)	27497-47-8									16.4		17.6	-1.2
1,3,5-Triphenylbenzene	C24H18 (1)	612-71-5	367.5		379.1	-11.6					224.6		223.4	1.2
Tetraphenylmethane	C25H20 (1)	630-76-2	397.8		398.7	-0.9					247.1		247.3	-0.2
1,3,6-Triphenyl-1,3,5-cycloheptatriene	C25H20 (2)	17760-68-8									273.9		273.6	0.3
9,10-Diphenylanthracene	C26H18 (1)	1499-10-1	465.6		414.2	51.4					308.7		256.9	51.8
Tetraphenylethylene	C26H20 (1)	632-51-9									311.5		311.3	0.2
1,1,1,2-Tetraphenylethane	C26H22 (1)	2294-94-2	365.3	ac	366.9	-1.7					223.0		272.4	-49.4
1,1,2,2-Tetraphenylethane	C26H22 (2)	632-50-8	357.3	ac	359.0	-1.7					216.0		220.9	-4.9
3-Phenyleicosane	C26H46 (1)	72557-70-1									-548.8		-543.1	-5.7
9-Phenyleicosane	C26H46 (2)						-476.0		-474.0	-2.0				
7-Hexadecylspiro[4,5]decane	C26H50 (1)	2307-06-4					-590.4		-596.4	6.0				
11-Cyclopentylheneicosane	C26H52 (1)	6703-82-8					-648.6		-645.2	-3.4				
3-Cyclohexyleicosane	C26H52 (2)	4443-57-6					-666.2		-670.7	4.5				
9-Cyclohexyleicosane	C26H52 (3)	4443-61-2					-674.1		-670.7	-3.4				
5-Butyldocosane	C26H54 (1)	55282-16-1	-587.6		-589.1	1.5	-713.5		-711.7	-1.8				

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 16

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
11-Butyldocosane	C26H54 (2)	13475-76-8	-593.4		-589.1	-4.3	-716.0		-711.7	-4.3				
11-Phenylheneicosane	C27H48 (1)	40775-09-5					-505.4		-499.6	-5.8				
11-Cyclohexylheneicosane	C27H54 (1)	6703-99-7					-689.4		-696.2	6.8				
9,9'-Bianthracene	C28H18 (1)	1055-23-8	454.3		449.4	4.9					326.2		290.4	35.8
9,9'-Biphenanthrene	C28H18 (2)	20532-03-0									212.8		268.6	-55.8
1,1,4,4-Tetraphenyl-1,3-butadiene	C28H22 (1)	1450-63-1									329.9		346.4	-16.5
1,2,3,4-Tetraphenyl-1,3-butadiene	C28H22 (2)	806-71-3									358.9		358.2	0.7
1,1,4,4-Tetraphenylbutane	C28H26 (1)	1483-64-3									163.3		162.3	1.0
(Tetra-p-tolylethylene)	C30H28 (1)	5831-43-6									171.5		157.3	14.2
1,1,2,2-Tetrakis(4-methylphenyl)ethane	C30H30 (1)	40673-57-2									73.6		75.3	-1.7
Cyclotriacontane	C30H60 (1)	297-35-8									-895.7		-878.6	-17.1
13-Phenylpentacosane	C31H56 (1)										-687.0		-689.5	2.5
13-Cyclohexylpentacosane	C31H62 (1)	3697-15-0					-792.7		-795.4	2.7				
11-Decylheneicosane	C31H64 (1)	55320-06-4	-705.8		-687.0	-18.8	-848.0		-834.7	-13.3				
Pentaphenylethane	C32H26 (1)	19112-42-6									381.2		366.5	14.7
Dotriacontane	C32H66 (1)	544-85-4	-697.2		-711.3	14.1	-859.4	SWS	-862.7	3.3	-968.3		-963.2	-5.1
Hexaphenylethane	C38H30 (1)	17854-07-8									511.8		512.1	-0.3
Rubrene (5,6,11,12-Tetraphenylnaphthacene	C42H28 (1)	517-51-1	780.9		723.0	57.9					620.3		470.3	150.0

Table 3. Carbon-Hydrogen compounds (CxHy): Enthalpy of formation (298 K), 17

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ

References

a. B. H. Justice and I. H. Carr, "The Heat of Formation of Propellant Ingredients," Dow Report No. AR-T0009-1S-67 (1967).
b. S. W. Benson and L. J. Garland, J. Phys. Chem. 95, 4915 (1991).
c. N. D. Lebedeva, V. L. Ryadnenko, N. N. Kiseleva, and L. F. Nazarova, Vses. Konf. Kalorim. (Rasshir. Tezisy Dokl.) 7th, 1, 91 (1977); from Chem. Abst. 92:75617q and Lias et al. and Lias et al.
d. W. V. Steele, R. D. Chirico, A. Nguyen, I. A. Hossenlopp, and N. K. Smith, "Determination of Ideal Gas Enthalpies of Formation for Key Compounds," in "Results from the Design Institute for Physical Property Data: Experimentl Results and Data Compilation Procedures," AIChE Symp. Ser. Vol. 86, No. 279 (1990), p. 138.
e. W. R. Roth, H.-W.Lennartz, E. Vogel, M. Leiendecker, and M. Oda, Chem. Ber. 119, 837 (1986).
f. 84ROT (private communication, W. R. Roth, in NIST SRD DB 25)
g. W. R. Roth, F.-G. Klarner, and H.-W. Lennartz, Chem. Ber. 113, 1818 (1980).
h. D. W. Rogers, O. A. Dagdagan, and N. L. Allinger, J. Am. Chem. Soc. 101, 671 (1979). ΔH of hydrogenation of the liquid was measured; the gas phase value was assumed to be the same. The derived ΔHf(gas) is probably accurate within 0.5 kcal/mol.
i. W. V. Steele and R. D. Chirico, J. Phys. Chem. Ref. Data 22, 377 (1993).
j. W. E. Billups et al., J. Am. Chem. Soc. 95, 7878 (1973); ref. 73BIL/CHO as quoted in NIST SRD DB 25.
k. J. E. Bartmess, J. Am. Chem. Soc. 104, 335 (1982; ref. 82BAR in Lias et al. T. Bally, D. Hasselmann, and K. Loosen, Helv. Chim. Acta 68, 345 (1985) report 47.0 kcal/mol for 20679-59-8
l. J. L. Jensen, Prog. Phys. Org. Chem. 12, 189 (1976).
m. N. L. Allinger, H. Dodziuk, D. W. Rogers, and S. N. Naik, Tetrahedron 38, 1593 (1982).
n. D. W. Rogers and K. Dejroonsgruang, J. Chem. Thermodyn. 21, 1115 (1989).
o. W. R. Roth and B. P. Scholz, Chem. Ber. 114, 3741 (198?); ref. 81ROT/SCH in Lias et al.
p. S. K. Pollack, B. C. Raine, and W. J. Hehre, J. Am. Chem. Soc. 103, 6308 (1981).
q. R. B. Turner and W. R. Meador, J. Am. Chem. Soc. 79, 4133 (1958); CA 52:1191h.
r. D. W. Rogers, K. Dejroonsgruang, S. D. Samuel, W. Fang, and Y. Zhao, J. Chem. Thermodyn. 24, 565 (1992).
s. M. P. Kozina, L. P. Timofeeva, S. M. Pinenova, V. A. Aleshna, et al., Russ J. Phys. Chem. 46, 1689 (1972), as quoted in Chem. Abst. 78:63105u.
t. R. Jochems, H. Dekker, C. Mosselman, and G. Somsen, J. Chem. Thermodyn. 15, 95 (1983).
u. H. E. Davis, N. L. Allinger, and D. W. Rogers, J. Org. Chem. 50, 3601 (1985); ref. 85DAV/ALL in Lias et al.
v. J. F. Liebman, L. A. Paquette, J. L. Peterson, and D. W. Rogers, J. Am. Chem. Soc. 108, 8267 (1986).
w. W. R. Roth, F.-G. Klarner, and H.-W. Lennartz, Chem. Ber. 113, 1818 (1980), gives 45 kcal/mol.
x. PNK error.
y. Misquoted in PNK.
z. N. Wakayama and H. Inokuchi, Bull. Chem. Soc. Jpn. 40, 2267 (1967). PNK quote 69.6 kcal/mol from an alternative source.
aa. Each cyclohexane attached to benzene ring must be in non-chair conformation, for 17-21 kJ/mol (4-5 kcal/mol) per ring.
ab. T. N. Nesterova, S. P. Verekin, S. Y. Karaseva, A. M. Rozhnov, and V. F. Tsyetkov, Russ. J. Phys. Chem. 58, 491 (1984); ref. 84NES/VER in Lias et al.
ac. H.-D. Beckhaus, B. Dogan, J. Schaetzer, S. Hellman, and C. Ruchardt, Chem. Ber. 123, 137 (1990).

L: S. G. Lias, J. E. Bartmess, J. F. Liebman, J. L. Holmes, R. D. Levin, and W. G. Mallard, "Gas-Phase Ion and Neutral Thermochemistry," J. Phys. Chem. Ref. Data, 17, Supplement No. 1 (
DH: E. S. Domalski and E. D. Hearing, "Estimation of the Thermodynamic Properties of C-H-N-O-S-Halogen Compounds at 298.15 K," J. Phys. Chem. Ref. Data 22, 805 (1993).
SWS: D. R. Stull, E. F. Westrum, Jr., and G. C. Sinke, The Chemical Thermodynamics of Organic Compounds (Krieger, 1987). These values are not in PNK and are of questionable reliabilit
P94: J. B. Pedley, Thermochemical Data and Structures of Organic Compounds, Vol. 1 (TRC Data Series, 1994).
*. The discrepancy represents stabilization from resonance between the aromatic ring and the double bond of the cyclohexene.

Table 4. Carbon-Hydrogen-Oxygen compounds (CxHyO): Enthalpy of formation (298 K), 1

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
Formaldehyce	CH2O (1)	50-00-0	-108.6				-170.7							
Paraformaldehyde	CH2O (2)	9002-81-7									-171.3		-171.5	0.2
Methanol	CH4O (1)	67-56-1	-201.5		-200.4	-1.1	-239.1		-238.9	-0.2				
Ethenone (Ketene)	C2H2O (1)	463-51-4	-47.5		-47.7	0.2	-67.9		-67.8	-0.1				
Acetaldehyde	C2H4O (1)	75-07-0	-166.1		-164.8	-1.3	-191.8		-192.0	0.2				
Oxirane (Ethylene oxide)	C2H4O (2)	75-21-8	-52.6		-54.4	1.8	-77.6		-80.8	3.2				
Ethenol	C2H4O	557-75-5	-125.5	L	-143.9	18.4								
Ethanol	C2H6O (1)	64-17-5	-235.2		-234.3	-0.9	-277.8	DH	-277.0	-0.8				
Dimethyl ether (Oxybismethane)	C2H6O (2)	115-10-6	-184.1		-183.3	-0.8	-203.3	P94	-202.1	-1.3				
2-Propenal (Acrolein)	C3H4O	107-02-8	-75.3	S	-67.4	-7.9								
1-Propen-1-one (Methyl ketene)	C3H4O	6004-44-0	-104.6	L	-104.6	-0.0								
Oxiranone (Cyclopropanone)	C3H4O	5009-27-8	16.8	L	16.7	0.0								
2-Propen-1-ol (Allyl alcohol)	C3H6O (1)	107-18-6	-124.5		-125.1	0.6	-171.8		-171.1	-0.7				
Propanal	C3H6O (2)	123-38-6	-185.6		-186.6	1.0	-215.3		-213.8	-1.5				
Acetone	C3H6O (3)	67-64-1	-217.3		-216.3	-1.0	-248.1		-248.5	0.4				
Methyloxirane (Propylene oxide)	C3H6O (4)	75-56-9	-94.7		-92.5	-2.2	-122.6		-120.5	-2.1				
Oxetane (Trimethylene oxide)	C3H6O (5)	503-30-0	-80.5		-83.7	3.2	-110.9	P94	-113.4	2.5				
(E)-Prop-1-en-ol	C3H6O	57642-95-2	-167.4	S	-176.1	8.8								
(Z)-Prop-1-en-ol	C3H6O	57642-96-3	-175.7	S	-171.5	-4.2								
Prop-1-en-2-ol (2-Hydroxypropene)	C3H6O	29456-04-0	-176.0	a	-184.5	8.5								
1-Propanol	C3H8O (1)	71-23-8	-255.1		-255.2	0.1	-302.6		-302.5	-0.1				
2-Propanol	C3H8O (2)	67-63-0	-272.8		-272.4	-0.4	-318.1		-316.7	-1.4				
Ethyl methyl ether (Methoxyethane)	C3H8O (3)	540-67-0	-216.4		-217.1	0.7								
Furan	C4H4O (1)	110-00-9	-34.9		-33.5	-1.4	-62.3		-60.2	-2.1				
But-1-yn-3-one	C4H4O	1423-60-5	65.3	L	65.3	0.0								
But-1-en-3-yn-2-ol	C4H4O	59095-55-5 *	82.8	G	82.4	0.4								
(E)-2-Butenal (Crotonaldehyde)	C4H6O (1)	4170-30-3	-100.6		-99.6	-1.0	-138.7		-133.5	-5.2				
Divinyl ether	C4H6O (2)	109-93-3	-13.6		-13.4	-0.2	-39.8		-38.5	-1.3				
2-Hydroxybutadiene	C4H6O	59120-04-6	-75.3	S	-85.4	10.0								
(E)-1-Hydroxy-1,3-butadiene	C4H6O	70411-98-2	-87.9	S	-87.0	-0.8								
(Z)-1-Hydroxy-1,3-butadiene	C4H6O	70415-58-6	-87.9	S	-82.4	-5.4								
2-Methyl-2-propenal	C4H6O	78-85-3	-117.2	S	-99.6	-17.6								
3-Buten-2-one	C4H6O	78-94-4	-138.1	S	-129.3	-8.8								
2-Methyl-1-propen-1-one	C4H6O	598-26-5	-133.9	S	-133.9	-0.0								
2,5-Dihydrofuran	C4H6O	1708-29-8	-66.9	S	-67.8	0.8								
2,3-Dihydrofuran	C4H6O	1191-99-7	-77.2	G	-109.6	32.4								
1,3-Butadien-2-ol	C4H6O	59120-04-6	-77.0	G	-85.4	8.4								

Table 4. Carbon-Hydrogen-Oxygen compounds (CxHyO): Enthalpy of formation (298 K), 2

Compound	Formula	CAS	Gas				Liquid				Solid			
	(PNK #)	Registry No.	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
(E)-1,2-Butadien-1-ol	C4H6O		-87.9	G	-28.5	-59.4								
(Z)-1,2-Butadien-1-ol	C4H6O		-90.0	G	-33.1	-56.9								
Cyclobutanone	C4H6O		-101.3	b	-101.3	0.0	-139.3	b	-141.0	1.7				
Butanal	C4H8O (1)	123-72-8	-204.8		-207.5	2.7	-239.2		-239.3	0.1				
2-Methylpropanal	C4H8O (2)	78-84-2	-215.8		-213.8	-2.0	-247.4		-246.4	-1.0				
2-Butanone (Methyl ethyl ketone)	C4H8O (3)	78-93-3	-238.7		-238.1	-0.6	-273.3		-270.3	-3.0				
Ethyl vinyl ether (Ethoxyethene)	C4H8O (4)	109-92-2	-140.8		-141.0	0.2	-167.4		-166.5	-0.9				
Ethyloxirane	C4H8O (5)	106-88-7					-168.9		-146.0	-22.9				
Tetrahydrofuran (Oxolane)	C4H8O (6)	109-99-9	-184.2		-184.5	0.3	-216.2		-215.5	-0.7				
2-Methoxy-1-propene	C4H8O (7)	116-11-0	-149.8	G	-147.7	-2.1	-177.3		-185.4	8.1				
(E)-2-Buten-2-ol	C4H8O		-230.1	G	-212.1	-18.0								
(Z)-2-Buten-2-ol	C4H8O	21451-76-3	-231.8	G	-212.1	-19.7								
1-Butanol	C4H10O (1)	71-36-3	-275.0		-276.1	1.1	-327.3		-328.0	0.7				
2-Methyl-1-propanol	C4H10O (2)	78-83-1	-283.9		-286.2	2.3	-334.7		-334.7	-0.0				
2-Butanol	C4H10O (3)	78-92-2	-292.9		-293.3	0.4	-342.6		-342.3	-0.3				
tert-Butyl alcohol	C4H10O (4)	75-65-0	-312.5		-311.7	-0.8	-359.2		-359.4	0.2	-365.9	DH	-359.4	-6.5
Diethyl ether	C4H10O (5)	60-29-7	-252.1		-251.0	-1.1	-279.3		-278.2	-1.1				
Methyl propyl ether	C4H10O (6)	557-17-5	-238.2		-238.1	-0.1	-266.0		-265.7	-0.3				
Methyl isopropyl ether	C4H10O (7)	598-53-8	-252.0		-251.9	-0.1	-278.7		-277.0	-1.7				
Cyclopentanone	C5H8O (1)	120-92-3	-192.1		-192.0	-0.1	-235.7		-238.1	2.4				
Dihydro-2H-pyran	C5H8O (2)	25512-65-6	-125.1		-125.1	0.0	-157.4		-157.3	-0.1				
(Z)-1,2-Epoxycyclopentane (6-Oxabicyclo[3.1.0]he	C5H8O (3)	285-67-6	-97.1	P94	-97.1	0.0	-131.0	P94	-131.0	-0.0				
3-Methyl-3-buten-2-one	C5H8O	814-78-8	-175.7	S	-161.5	-14.2								
3-Penten-2-one	C5H8O	625-33-2	-175.7	S	-161.5	-14.2								
(E)-2-Pentenal	C5H8O	764-39-6	-125.5	L	-119.7	-5.9								
2-Methyl-2-butenal	C5H8O	497-03-0	-138.1	L	-131.8	-6.3								
1-Penten-3-one	C5H8O	1629-58-9	-138.1	L	-151.0	13.0								
Cyclopropyl-methyl-ketone	C5H8O	765-43-5	-117.2	L	-107.5	-9.6								
Diethyl ketone	C5H10O (1)	96-22-0	-257.9		-259.8	1.9	-296.5		-292.0	-4.5				
Methyl propyl ketone	C5H10O (2)	107-87-9	-259.0		-259.0	-0.0	-297.3		-295.8	-1.5				
Isopropyl methyl ketone	C5H10O (3)	563-80-4	-262.5		-261.9	-0.6	-299.4		-300.6	1.2				
Cyclopentanol	C5H10O (4)	96-41-3	-242.6		-242.7	0.1	-300.1		-299.2	-0.9				
Tetrahydro-2H-pyran (Oxane)	C5H10O (5)	142-68-7	-223.4		-225.5	2.1	-258.3		-259.0	0.7				
Pentanal	C5H10O (6)	110-62-3	-228.5		-228.4	-0.1	-267.3		-264.8	-2.5				
Propyl vinyl ether	C5H10O (7)	764-47-6	-161.6		-161.9	0.3	-190.9		-192.0	1.1				
3,3-Dimethyloxetane	C5H10O (8)	6921-35-3	-148.2		-146.9	-1.3	-182.2		-181.6	-0.6				
Isopropyl vinyl ether	C5H10O (9)	926-65-8	-173.8		-179.1	5.3	-205.1		-206.3	1.2				
2-Methyl-3-buten-2-ol	C5H10O	115-18-4	-125.5	L	-125.5	-0.0								
3-Methyl-2-buten-2-ol	C5H10O	34454-78-9	-241.0	G	-251.9	10.9								
2-Ethoxy-1-propene	C5H10O	926-66-9	-181.6	G,c	-181.6									

Table 4. Carbon-Hydrogen-Oxygen compounds (CxHyO): Enthalpy of formation (298 K), 3

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
(E)-2-Methoxy-2-butene	C5H10O	25125-84-2	-166.9	G	-179.9	13.0								
1-Pentanol	C5H12O (1)	71-41-0	-294.7		-297.1	2.4	-351.6		-353.5	1.9				
2-Pentanol	C5H12O (2)	6032-29-7	-312.7		-314.2	1.5	-365.2		-367.8	2.6				
3-Pentanol	C5H12O (3)	584-02-1	-317.2		-314.2	-3.0	-368.9		-367.8	-1.1				
2-Methyl-1-butanol	C5H12O (4)	137-32-6	-302.0		-303.8	1.8	-356.6		-357.9	1.3				
3-Methyl-1-butanol	C5H12O (5)	123-51-3	-301.0		-303.8	2.8	-356.4		-357.9	1.5				
2-Methyl-2-butanol	C5H12O (6)	75-85-4	-330.8		-329.3	-1.5	-379.5		-382.6	3.1				
3-Methyl-2-butanol	C5H12O (7)	598-75-4	-315.2		-317.6	2.4	-366.6		-369.8	3.2				
t-Butyl methyl ether	C5H12O (8)	1634-04-4	-283.5		-287.9	4.4	-313.6		-316.7	3.1				
2,2-Dimethyl-1-propanol	C5H12O (9)	75-84-3					-399.4		-366.1	-33.3				
Methyl butyl ether	C5H12O (10)	628-28-4	-258.1		-259.0	0.9	-290.6		-291.2	0.6				
Ethyl propyl ether	C5H12O (11)	628-32-0	-272.2		-272.0	-0.2	-303.6		-303.8	0.2				
Phenol	C6H6O (1)	108-95-2	-96.4		-95.8	-0.6	-156.4	DH	-159.8	3.5	-165.1		-168.2	3.1
Vinylfuran (2-Ethenylfuran)	C6H6O (2)	1487-18-9	27.8		25.1	2.7	-10.3		-9.2	-1.1				
Cyclopentene-1-methanol	C6H10O (1)	1120-80-5					34.4		-207.9	242.3				
2-Methylene cyclopentanol	C6H10O (2)	20461-31-8					46.9		-305.4	352.3				
2-Methylcyclopentanone	C6H10O (3)	1120-72-5					-265.2		-270.7	5.5				
Cyclohexanone	C6H10O (4)	108-94-1	-227.7	b	-227.6	-0.1	-272.8	b	-274.5	1.7				
7-Oxabicyclo[2.2.1]heptane	C6H10O (5)	279-49-2	-184.1	S	-184.1	-0.0	-223.9		-223.8	-0.1				
1-Methoxycyclopentene	C6H10O (6)	1072-59-9	-126.8	G	-132.6	5.9	-167.8		-182.0	14.2				
(Z)-1,2-Epoxycyclohexane (7-Oxabicyclo[4.1.0]hep	C6H10O (7)	286-45-3	-125.6	P94	-243.5	117.9	-166.1	P94	-265.7	99.6				
2-Hexanone	C6H12O (1)	591-78-6	-279.8		-279.9	0.1	-322.0		-321.3	-0.7				
3,3-Dimethyl-2-butanone	C6H12O (2)	75-97-8	-290.7		-287.4	-3.3	-328.6		-326.4	-2.2				
3-Hexanone	C6H12O (3)	589-38-8	-278.3		-280.7	2.4	-320.2		-317.6	-2.6				
2-Methyl-3-pentanone	C6H12O (4)	565-69-5	-286.1		-283.7	-2.4	-325.9		-322.4	-3.5				
(Z)-2-Methylcyclopentanol	C6H12O (5)	25144-05-2					-345.5		-331.4	-14.1				
Cyclohexanol	C6H12O (6)	108-93-0	-290.0	S	-290.4	0.4	-348.2		-350.2	2.0				
Butyl vinyl ether	C6H12O (7)	111-34-2	-184.5		-182.8	-1.7	-218.8		-217.6	-1.2				
4-Methyl-2-Pentanone	C6H12O		-348.0	f	-286.6	-61.4	-388.7	SWS	-325.7	-63.0				
Hexanal	C6H12O	66-25-1	-246.9	S	-249.4	2.5								
Hexanol	C6H14O (1)	25917-35-5	-315.8		-318.0	2.2	-377.5		-379.1	1.6				
Dipropyl ether	C6H14O (2)	111-43-3	-292.9		-292.9	-0.0	-328.8		-329.3	0.5				
Diisopropyl ether	C6H14O (3)	108-20-3	-319.2		-320.5	1.3	-351.5		-351.9	0.4				
2-Methyl-3-pentanol	C6H14O (4)	565-67-3					-396.4		-400.0	3.6				
2-Hexanol	C6H14O (5)	626-93-7	-334.7	S	-335.1	0.4	-392.0		-393.3	1.3				
4-Methyl-2-pentanol	C6H14O (6)	108-11-2					-394.7		-400.0	5.3				
3-Hexanol	C6H14O (7)	623-37-0					-392.4		-393.3	0.9				
2-Methyl-2-methoxy-butane	C6H14O (8)		-306.7	P94	-294.6	-12.1	-341.8	P94	-345.8	4.0				
t-Butyl ethyl ether (2-Ethoxy-2-methylpropane)	C6H14O (9)	637-92-3	-313.8	P94	-328.4	14.6								
Butyl ethyl ether	C6H14O	628-81-9	-292.9	L	-292.9	-0.0								

Table 4. Carbon-Hydrogen-Oxygen compounds (CxHyO): Enthalpy of formation (298 K), 4

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
s-Butyl ethyl ether	C6H14O	2679-87-0	-313.8	L	-306.7	-7.1								
Benzaldehyde	C7H6O (1)	100-52-7	-36.7		-37.2	0.5	-87.0		-87.9	0.9				
2,4,6-Cycloheptatrien-1-one	C7H6O (2)	539-80-0	43.9		34.3	9.6	-10.0		-10.0	0.0				
Benzyl alcohol	C7H8O (1)	100-51-6	-100.4		-95.8	-4.6	-160.7		-159.8	-0.9				
2-Methylphenol (o-Cresol)	C7H8O (2)	95-48-7	-125.5	d	-126.4	0.8					-204.6		-198.3	-6.3
3-Methylphenol (m-Cresol)	C7H8O (3)	108-39-4	-132.3		-128.4	-3.9	-194.0		-196.5	2.5				
4-Methylphenol (p-Cresol)	C7H8O (4)	106-44-5	-125.4		-128.4	3.0					-199.3		-204.6	5.3
Methoxybenzene (Anisole)	C7H8O (5)	100-66-3	-67.9		-66.9	-1.0	-114.8		-118.0	3.2				
3,5-Cycloheptadien-1-one	C7H8O	1121-65-9	-7.1	S	-6.7	-0.4								
Bicyclo[2.2.1]heptan-2-one	C7H10O (1)	497-38-1	-170.6	#	-171.5	0.9					-219.5		-225.9	6.4
Bicyclo[2.2.1]heptan-7-one	C7H10O (2)	10218-02-7	-134.1	#	-134.3	0.2					-181.3		-181.2	-0.1
2-Methylcyclohexanone	C7H12O (1)	583-60-8					-288.1		-307.1	19.0				
Cycloheptanone	C7H12O (2)	502-42-1	-247.5		-247.7	0.2	-299.4		-299.2	-0.2				
1-Cyclohexene-1-methanol	C7H12O (3)	4845-04-9					-382.6		-256.5	-126.1				
2-Methylenecyclohexanol	C7H12O (4)	4065-80-9					-277.6		-356.5	78.9				
1-Methoxycyclohexene	C7H12O (7)	931-57-7	-164.8	G	-161.1	-3.8	-210.8		-219.2	8.4				
(Z)-1,2-Epoxy-cycloheptane (8-Oxabicyclo[5.1.0]o	C7H12O (8)	286-45-3	-152.3	P94	-152.3	-0.0	-197.5	P94	-197.5	-0.0				
Cyclohexanecarboxaldehyde	C7H12O	2043-61-0	-235.1	S	-234.7	-0.4								
Heptanal	C7H14O (1)	111-71-7	-263.8		-270.3	6.5	-311.5		-315.9	4.4				
tert-Butyl ethyl ketone	C7H14O (2)	564-04-5	-313.7		-309.2	-4.5	-356.1		-348.1	-8.0				
Diisopropyl ketone	C7H14O (3)	565-80-0	-311.3		-300.8	-10.5	-352.9		-348.1	-4.8				
Cyclohexanemethanol	C7H14O (4)	100-49-2					-378.1		-368.2	-9.9				
(Z)-2-Methylcyclohexanol	C7H14O (5)	7443-70-1	-327.0		-321.3	-5.7	-390.2		-382.3	-7.9				
(E)-2-Methylcyclohexanol	C7H14O (6)	7443-52-9	-352.5		-321.3	-31.2	-415.7		-382.4	-33.3				
(Z)-3-Methylcyclohexanol	C7H14O (7)	5454-79-5	-350.9		-321.3	-29.6	-416.1		-382.4	-33.7				
(E)-3-Methylcyclohexanol	C7H14O (8)	7443-55-2	-329.1		-321.3	-7.8	-394.4		-382.3	-12.1				
(Z)-4-Methylcyclohexanol	C7H14O (9)	7731-28-4	-347.5		-321.3	-26.2	-413.2		-382.3	-30.9				
(E)-4-Methylcyclohexanol	C7H14O (10)	7731-29-5	-367.2		-321.3	-45.9	-433.3		-382.4	-50.9				
1-Methylcyclohexanol	C7H14O	590-67-0	-359.8	S	-329.7	-30.1								
3-Heptanone	C7H14O	106-35-4	-297.1	S	-301.7	4.6								
2-Heptanone	C7H14O	110-43-0	-301.2	S	-300.8	-0.4								
4-Heptanone	C7H14O	123-19-3	-301.2	S	-301.7	0.4								
1-Heptanol	C7H16O (1)	111-70-6	-336.4		-338.9	2.5	-403.3		-404.6	1.3				
tert-Butyl isopropyl ether	C7H16O (2)	17348-59-3	-357.6		-356.5	-1.1	-392.8		-391.6	-1.2				
2-Heptanol	C7H16O	543-49-7	-355.6	S	-356.1	0.4								
3-Heptanol	C7H16O	589-82-2	-355.6	S	-356.1	0.4								
4-Heptanol	C7H16O	589-55-9	-355.6	S	-356.1	0.4								
Phenyl ethenone (Phenyl ketene)	C8H6O	3496-32-0	25.1	L	24.7	0.4								
Benzofuran	C8H6O	271-89-6	25.1	L	25.5	-0.4								
1-Phenylethanone (Acetophenone)	C8H8O (1)	98-86-2	-86.7		-86.6	-0.1	-142.5		-144.8	2.3				

Table 4. Carbon-Hydrogen-Oxygen compounds (CxHyO): Enthalpy of formation (298 K), 5

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
Phenyl vinyl ether	C8H8O (2)	766-94-9	22.7		39.7	-17.0	-26.2		-26.4	0.2				
1-Phenylethenol	C8H8O		-46.0	G *	-43.1	-2.9								
2-Ethylphenol	C8H10O (1)	90-00-6	-145.2		-147.7	2.5	-208.8		-222.4	13.6				
3-Ethylphenol	C8H10O (2)	620-17-7	-146.1		-147.7	1.6	-214.3		-222.4	8.1				
4-Ethylphenol	C8H10O (3)	123-07-9	-144.1		-147.7	3.6					-224.4		-231.8	7.4
2,3-Dimethylphenol (2,3-Xylenol)	C8H10O (4)	526-75-0	-157.2		-156.5	-0.7					-241.2		-232.2	-9.0
2,4-Dimethylphenol	C8H10O (5)	105-67-9	-162.9		-159.0	-3.9	-228.7		-233.1	4.4				
2,5-Dimethylphenol	C8H10O (6)	95-87-4	-161.6		-159.0	-2.6					-246.6		-234.7	-11.9
2,6-Dimethylphenol	C8H10O (7)	576-26-1	-161.8		-156.9	-4.9					-237.4		-228.4	-9.0
3,4-Dimethylphenol	C8H10O (8)	95-65-8	-156.6		-158.6	2.0					-242.3		-238.5	-3.8
3,5-Dimethylphenol	C8H10O (9)	108-68-9	-161.5		-161.1	-0.4					-244.4		-241.0	-3.4
Ethoxybenzene (Phenetole)	C8H10O (10)	103-73-1	-101.6		-100.8	-0.8	-152.6		-156.1	3.5				
1-Methoxy-3-methylbenzene	C8H10O (11)	100-84-5	-104.1		-99.6	-4.5	-155.6		-154.6	-1.0				
(Methoxymethyl)-benzene	C8H10O	538-86-3	-75.3	S	-101.3	25.9								
(Z)-Bicyclo[3.3.0]octan-2-one	C8H12O (1)	19915-11-8	-230.1		-217.1	-13.0	-284.5		-269.9	-14.6				
(E)-Bicyclo[3.3.0]octan-2-one	C8H12O (2)	29365-79-5	-206.7		-221.8	15.1	-260.2		-273.6	13.4				
2,5-Endo-ethylene cyclohexanone	C8H12O (3)	55973-22-3	-222.2	P94	-233.5	11.3	-274.0	P94	-271.1	-2.9				
Bicyclo[2.2.2]octanone	C8H12O	2716-23-6	-230.1	S	-230.1	-0.0								
2-Ethyl-2-hexenal	C8H14O (1)	645-62-5					-261.2		-225.9	-35.3				
Cyclooctanone	C8H14O (2)	502-49-8	-271.6		-272.4	0.8	-326.0		-325.9	-0.1	-323.4		-323.4	0.0
3-Oxabicyclo[3.2.2]nonane	C8H14O (3)	283-27-2	-222.5		-222.6	0.1					-275.6		-275.3	-0.3
(Z)-1,2-Epoxycyclooctane	C8H14O (4)		-165.3	P94	-165.3	-0.0	-212.6	P94	-212.5	-0.0				
2-Ethylhexanal	C8H16O (1)	123-05-7	-299.6		-297.5	-2.1	-348.5		-348.5	0.0				
2,2,4-Trimethyl-3-pentanone	C8H16O (2)	5857-36-3	-338.3		-343.1	4.8	-381.6		-385.3	3.7				
(1a,3a,5a)-3,5-Dimethylcyclohexanol	C8H16O (3)	767-13-5					-424.3	P94	-414.6	-9.6				
(1b,3a,5a)-3,5-Dimethylcyclohexanol	C8H16O (4)	17373-17-0					-485.0	P94	-414.6	-70.4				
(1a,3a,5b)-3,5-Dimethylcyclohexanol	C8H16O (5)	767-14-6					-509.7	P94	-414.6	-95.1				
2-Octarone	C8H16O	111-13-7	-322.2	S	-321.7	-0.4								
3-Octarone	C8H16O						-382.8	SWS	-368.6	-14.2				
4-Octarone	C8H16O	589-63-9	-318.0	S	-322.6	4.6								
Octanal (Caprylaldehyde)	C8H16O	124-13-0	-279.5	e	-291.2	11.7								
1-Octanol	C8H18O (1)	111-87-5	-355.5		-359.8	4.3	-426.5		-430.1	3.6				
2-Ethyl-1-hexanol	C8H18O (2)	104-76-7	-365.3		-363.2	-2.1	-432.8		-432.2	-0.6				
Dibutyl ether	C8H18O (3)	142-96-1	-333.4		-334.7	1.3	-377.9		-380.3	2.4				
Di-sec-butyl ether	C8H18O (4)	6863-58-7	-360.9		-362.3	1.4	-401.5		-402.9	1.4				
Di-tert-butyl ether	C8H18O (5)	6163-66-2	-362.0		-361.9	-0.1	-399.6		-400.8	1.2				
Butyl t-butyl ether	C8H18O (6)		-361.1	P94	-363.6	2.5	-403.3	P94	-405.8	2.5				
i-Butyl t-butyl ether	C8H18O (7)		-369.0	P94	-373.6	4.6	-409.2	P94	-412.5	3.3				
s-Butyl t-butyl ether	C8H18O (8)		-380.0	P94	-367.4	-12.6	-420.5	P94	-405.6	-14.9				
1-Phenyl-2-propanone	C9H10O (1)	103-79-7	-100.7		-105.0	4.3	-151.9		-151.9	-0.0				
1-Phenyl-1-propanone	C9H10O (2)	93-55-0	-108.7		-108.4	-0.3	-167.2		-166.5	-0.7				

Table 4. Carbon-Hydrogen-Oxygen compounds (CxHyO): Enthalpy of formation (298 K), 6

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
3,4-Dihydro-2H-1-benzopyran	C9H10O (3)	493-08-3	-82.4	P94	-82.4	0.0					-138.9	P94	-138.9	-0.0
3,4-Dihydro-1H-2-benzopyran	C9H10O (4)	493-05-0	-63.1	P94	-63.2	0.1					-120.2	P94	-120.1	-0.1
3-Phenyl-2-propen-1-ol	C9H10O	104-54-1	-29.3	S	-29.7	0.4								
3-Phenylpropanal	C9H10O	1335-10-0	-71.1	S	-72.0	0.8								
2-Indanol	C9H10O	4254-29-9	-133.9	S	-125.9	-7.9								
a-Ethenyl-benzenemethanol	C9H10O	4393-06-0	-25.1	S	-24.3	-0.8								
2-(2-Methylphenyl)ethanal	C9H10O	69380-02-5	-83.7	S	-83.7									
2-Isopropylphenol	C9H12O (1)	88-69-7	-182.2		-172.4	-9.8	-233.7		-249.2	15.5	-246.6		-244.8	-1.8
3-Isopropylphenol	C9H12O (2)	618-45-1	-196.0		-174.5	-21.5	-252.5		-249.2	-3.3	-263.0		-251.0	-12.0
4-Isopropylphenol	C9H12O (3)	99-89-8	-209.4		-174.5	-34.9	-265.9		-249.2	-16.7	-279.7		-251.0	-28.7
(Z)-Octahydro-2H-inden-2-one	C9H14O (1)	5689-04-3	-249.6		-250.2	0.6	-307.1		-307.5	0.4				
(E)-Octahydro-2H-inden-2-one	C9H14O (2)	16484-17-6	-249.2		-250.2	1.0	-305.3		-307.5	2.2				
Cyclononanone	C9H16O	3350-30-9	-279.7	b	-279.5	-0.2	-332.9	DH	-334.3	1.5	-334.9	b	-334.7	-0.2
Dibutyl ketone	C9H18O (1)	502-56-7	-344.9		-343.5	-1.4	-398.2		-394.1	-4.1				
Di-tert-butyl ketone	C9H18O (2)	815-24-7	-345.8		-345.6	-0.2	-391.1		-392.0	0.9				
Diisobutyl ketone	C9H18O (3)	108-83-8	-357.6		-356.9	-0.7	-405.8		-402.9	-2.9				
2-Nonanone	C9H18O (4)	821-55-6	-340.7		-342.7	2.0	-397.2		-397.9	0.7				
1-Nonanol	C9H20O (1)	143-08-8	-376.3		-380.7	4.4	-453.4		-455.6	2.2				
3,5,5-Trimethyl-1-hexanol	C9H20O (2)	3452-97-9					-456.5		-470.3	13.8				
Pentyl t-butyl ether	C9H20O (3)	10100-95-5	-380.6	P94	-384.5	3.9								
1-Naphthol (1-Naphthalenol)	C10H8O (1)	90-15-3	-29.9		-28.9	-1.0					-121.0		-120.5	-0.5
2-Naphthol	C10H8O (2)	135-19-3	-30.0		-28.9	-1.1					-124.2		-120.5	-3.7
11-Oxabicyclo[4.4.1]undeca-1,3,5,7,9-pentaene	C10H8O (3)	4759-11-9	199.9		200.4	-0.5	139.1		138.9	0.2	119.5		119.7	-0.2
1,4-Dihydro-1,4-epoxynaphthalene	C10H8O (4)	573-57-9									61.9	P94	61.9	0.0
3-Phenylcyclobutenone	C10H8O										28.0	SWS	28.0	0.0
1-Tetralone	C10H10O (1)	529-34-0									-209.6	P94	-226.8	17.2
4-Phenyl-3-buten-2-one	C10H10O	122-57-6	-25.1	S	-33.9	8.8								
3-Phenylcyclobutanone	C10H10O						-56.5	SWS	-33.1	-23.4				
1-Phenyl-1-butanone	C10H12O (1)	495-40-9	-128.2		-129.3	1.1	-188.9		-192.0	3.1				
1,2,3,4-Tetrahydro-1-naphthol	C10H12O (2)	529-33-9									-241.4		-253.6	12.2
5,6,7,8-Tetrahydro-1-naphthol	C10H12O (3)	529-35-1									-285.3		-271.5	-13.8
Cyclopropyl phenylmethanol	C10H12O	1007-03-0	-21.0	S	-20.9	-0.0								
1-Phenyl cyclopropane-1-methanol	C10H12O	31729-66-5	-16.7	S	-14.2	-2.5								
2-Isopropyl-5-methylphenol (Thymol)	C10H14O (1)	89-83-8	-218.5		-205.0	-13.5					-309.7		-281.2	-28.5
3-Isopropyl-2-methylphenol	C10H14O (2)	4371-48-6	-241.5		-202.5	-39.0	-295.9		-284.1	-11.8				
4-Isopropyl-2-methylphenol	C10H14O (3)	1740-97-2	-243.6		-205.0	-38.6	-300.1		-285.8	-14.3				
5-Isopropyl-2-methylphenol	C10H14O (4)	499-75-2	-228.5		-205.0	-23.5	-287.5		-285.8	-1.7				
2-Isopropyl-6-methylphenol	C10H14O (5)	3228-04-4	-235.6		-202.9	-32.7	-287.5		-285.8	-1.7				
Adamantan-2-one (Tricyclo[3.3.1.1^3,7]-decanone)	C10H14O (5)	700-58-3	-230.6		-230.5	-0.1					-311.0		-310.9	-0.1

Table 4. Carbon-Hydrogen-Oxygen compounds (CxHyO): Enthalpy of formation (298 K), 7

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one (Camphor)	C10H16O (1)	76-22-2	-267.5		-263.6	-3.9					-319.4		-313.8	-5.6
(Z)-8-Methyl-octahydro-2H-inden-2-one	C10H16O (2)		-287.0	P94	-282.4	-4.6					-348.1	P94	-348.1	-0.0
(E)-8-Methyl-octahydro-2H-inden-2-one	C10H16O (3)		-275.3	P94	-282.4	7.1	-333.5	P94	-343.5	10.0				
Adamantan-1-ol	C10H16O (4)	768-95-6	-311.0		-310.9	-0.1					-397.6		-409.6	12.0
Adamantan-2-ol	C10H16O (5)	700-57-2	-299.3		-302.5	3.2					-388.0		-377.8	-10.2
(E)-9-Hydroxy-decahydronaphthalene	C10H18O (1)										-444.3	P94	-478.6	34.3
Cyclodecanone	C10H18O	1502-06-3	-305.1	b	-305.0	-0.0	-363.4	b	-364.8	1.4				
2,2,5,5-Tetramethyl-3-hexanone	C10H20O (1)	868-91-7	-393.9		-400.0	6.1	-442.7		-446.4	3.7				
1-Decanol	C10H22O (1)	112-30-1	-396.4		-401.7	5.3	-478.1		-481.2	3.1				
2-Methoxynaphthalene	C11H10O (1)	93-04-9									-97.9		-102.1	4.2
2,2-Dimethyl-2H-1-Benzopyran	C11H12O	2513-25-9	-41.8	S	-41.4	-0.4								
(E)-4-(3-Methylphenyl)-but-3-en-2-one	C11H12O	15753-84-1	-66.9	S	-66.5	-0.4								
(E)-4-(2-Methylphenyl)-but-3-en-2-one	C11H12O	16927-82-5	-54.4	S	-64.0	9.6								
3-Methyl-1-phenyl-1-butanone	C11H14O (1)	582-62-7	-160.7		-160.2	-0.5	-220.2		-224.3	4.1				
2,2-Dimethyl-1-phenyl-1-propanone	C11H14O (2)	938-16-9					-208.9		-227.2	18.3				
1-(2,4,5-Trimethylphenyl)-ethanone	C11H14O (3)	2040-07-5	-189.0		-179.5	-9.5	-252.2		-251.4	-0.8				
1-(2,4,6-Trimethylphenyl)-ethanone	C11H14O (4)	1667-01-2	-204.9		-179.5	-25.4	-267.2		-251.4	-15.8				
1-tert-Butyl-4-methoxybenzene	C11H16O	5396-38-3	-173.6	S	-171.1	-2.5								
Cycloundecanone	C11H20O	878-13-7	-322.0	b	-322.2	0.2	-386.4	b	-387.9	1.5				
Dipentyl ketone	C11H22O (1)	927-49-1	-387.4		-385.3	-2.1	-448.1		-445.2	-2.9				
2,2,6,6-Tetramethyl-4-heptanone	C11H22O (2)	4436-99-1	-421.2		-428.0	6.8	-474.1		-479.5	5.4				
1-Methoxydecane	C11H24O (1)	7289-52-3	-381.1		-384.5	3.4	-443.4		-444.3	0.9				
1-Undecanol	C11H24O (2)	112-42-5	-422.2	SWS	-422.6	0.4	-504.8		-506.7	1.9				
Dibenzofuran	C12H8O (1)	132-64-9	83.4		83.7	-0.3					-5.3		-5.0	-0.3
Diphenyl ether	C12H10O (1)	101-84-8	52.0		51.5	0.5	-14.9		-15.1	0.2	-32.1		-25.1	-7.0
2-Ethoxynaphthalene	C12H12O (1)	93-18-5									-134.0		-123.0	-11.0
1-Adamantyl methyl ketone	C12H18O (4)	1660-04-4	-298.3	P94	-293.3	-5.0					-382.4	P94	-389.1	6.7
Cyclododecanone	C12H22O	830-13-7	-349.1	b	-348.9	-0.2	-414.6	DH	-415.9	1.3	-431.3	b	-431.4	0.0
2-Dodecanone	C12H24O (1)	6175-49-1	-404.3		-405.4	1.1	-476.1		-474.5	-1.6				
1-Dodecanol	C12H26O (1)	112-53-8	-436.6		-443.5	6.9	-528.5		-532.2	3.7				
Dibenzopyran (Xanthene)	C13H10O (1)	229-95-8	48.4		49.4	-1.0					-63.8		-63.6	-0.2
Diphenylmethanone (Benzophenone)	C13H10O (2)	119-61-9	54.9		56.1	-1.2	-16.3	DH	0.0	-16.3	-34.5		-39.7	5.2
6,8-Dimethyl-7H-benzocyclohepten-7-one	C13H12O (2)	2484-16-4	-2.3		-2.5	0.2					-80.5		-80.3	-0.2
Diphenylmethanol (Benzhydrol)	C13H12O										-105.4	SWS	-105.4	
7-Phenyl-bicyclo[3.2.0]hept-2-en-6-ol	C13H14O	64353-61-3	71.1	S	72.0	-0.8								
1-tert-Butyl-4-(2-propynyloxy)-benzene	C13H16O	48144-15-6	62.8	S	62.8	0.0								
1-Tridecanol	C13H28O (1)	112-70-9									-599.4		-594.5	-4.9
Tri-t-butyl-methanol	C13H28O (2)	41902-42-5	-410.0	P94	-473.6	63.6					-469.9	P94	-528.9	59.0
Diphenyl ethenone	C14H10O	525-06-4	104.6	L	105.4	-0.8								

Table 4. Carbon-Hydrogen-Oxygen compounds (CxHyO): Enthalpy of formation (298 K), 8

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
9(10H)-Anthracenone (Dibenzocyclohexanone)	C14H10O	90-44-8	29.3	L	30.1	-0.8								
4-Methylbenzophenone	C14H12O (1)	134-84-9									-77.8		-76.1	-1.7
1,2-Diphenylethanone (Benzylphenyl ketone)	C14H12O (2)	451-40-1	22.3		24.7	-2.4					-71.0		-84.1	13.1
Diamantanone	C14H18O (1)	30545-23-4	-236.5		-236.4	-0.1					-339.6		-339.7	0.1
Diamantan-1-ol	C14H20O (1)	30545-19-8	-310.9	P94	-315.1	4.2					-428.9	P94	-446.0	17.2
Diamantan-3-ol	C14H20O (2)	30545-24-5	-297.5	P94	-304.2	6.7					-413.8	P94	-433.5	19.7
Diamantan-4-ol	C14H20O (3)	30651-03-7	-317.1	P94	-315.1	-2.1					-434.7	P94	-446.0	11.3
1-Tetradecanol	C14H30O (1)	112-72-1	-527.4		-485.3	-42.1	-580.6		-583.2	2.6	-629.6		-623.8	-5.8
Diphenylcyclcpropenone	C15H10O (1)	886-38-4	552.5		553.5	-1.0					411.1		410.9	0.2
4-Ethylbenzophenone	C15H14O (1)	18220-90-1					-64.3		-62.6	-1.7				
Dibenzyl ketone (1,3-Diphenylpropan-2-one)	C15H14O (2)	102-04-5	5.1		6.3	-1.2					-84.0		-86.2	2.2
2,3,4-Trimethyl-indeno[2,1-b]pyran	C15H14O (3)	10435-68-4	2.1	P94	64.4	-62.3					-137.7	P94	-23.0	-114.6
Cyclopentadecanone	C15H28O (1)	502-72-7	-414.5		-414.6	0.1					-491.9		-491.6	-0.3
1-Pentadecanol	C15H32O (1)	629-76-5									-658.2		-653.1	-5.1
8,9,10,11-Tetrahydro-6,12-methano-7H-benzo-cycloundecene-14-one	C16H16O (2)	25401-39-2	137.1		137.2	-0.1					50.9		51.0	-0.1
4-Isopropylbenzophenone	C16H16O (1)						-118.6	P94	-89.4	-29.2	-118.8	SWS	-122.6	3.8
1-Hexadecanol	C16H34O (1)	36653-82-4	-517.0		-527.2	10.2					-686.5		-682.4	-4.1
4-tert-Butylbenzophenone	C17H18O (1)	22679-54-5					-135.6		-119.5	-16.1				
2-Cycloheptadecen-1-one	C17H30O (1)		-408.3		-407.9	-0.4					-484.0		-483.7	-0.3
Cycloheptadecanone	C17H32O (1)	3661-77-6	-460.3		-460.2	-0.1					-536.0		-536.0	-0.0
6-Phenylindeno[2,-b]pyran (6-Phenyl-2,3-benzoox	C18H12O (1)		270.7	P94	270.7	0.0					128.0	P94	128.1	-0.0
Triphenylmethanol	C19H16O (1)	76-84-6									-2.5		-3.3	0.8
1,1'-Diadamantyl ketone	C21H30O (1)	38256-01-8	-367.8	P94	-298.3	-69.5					-477.0	P94	-484.5	7.5
Tris(4-methylphenyl)-methanol	C22H22O (1)	3247-00-5									-67.4		-112.5	45.1
2,4,6-Triisopropylbenzophenone	C22H28O (1)	33574-11-7	-188.5		-193.7	5.2					-304.5		-294.6	-9.9
3',5'-Diisopropyl-4,4-dimethyl-3-phenyl-1,2-benzocyclobuten-3-ol	C22H28O (2)	33574-16-2	-101.8		-101.7	-0.1					-218.8		-218.8	0.0
7,8,9,10,11,12,13,14,15,16,17,18-dodecahydro-6,19-methanobenzocyclooctadecen-21-one	C23H30O (1)	25401-43-8	-159.8		-159.4	-0.4					-263.2		-263.2	-0.0

Table 4. Carbon-Hydrogen-Oxygen compounds (CxHyO): Enthalpy of formation (298 K), 9

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ

Notes and References

*: Also Registry No. 103095-52-8

#: These two bicyclic ketones probably should have separate RSCs.

a: 84TUR/HAN: F. Turecek and V. Hanus, Org. Mass Spectrom. 19, 631 (1984).

b: 72WOL: G. Wolf, Helv. Chim. Acta 55, 1446 (1972).

c: Calculated by Guthrie (G).

d: 79KUD/KJD: S. A. Kudchadker, A. P. Kudchadker, R. C. Wilhoit, and B. J. Zwolinski, Thermochim. Acta, 30, 319 (1979).

e: 66GEI/RAT: G. Geiseler, N. Ratlevszh, K. Ebster, and I. Ziegel, Ber. Bunsenges. Phys. Chem. 70, 221 (1966)

f: Gas phase value calculated from liquid value and ΔHvap recommended by V. Majer and V. Svoboda, "Enthalpies of Vaporization of Organic Compounds," Blackwell Scientific Publs., 1985

S: S. E. Stein, "NIST Structures and Properties, NIST-SRD DB 25, Version 2.0 (January 1994).

L: S. G. Lias, J. E. Bartmess, J. F. Liebman, J. L. Holmes, R. D. Levin, and W. G. Mallard, "Gas-Phase Ion and Neutral Thermochemistry," J. Phys. Chem. Ref. Data, 17, Supplement No. 1 (1988).

G: J. P. Guthrie, "Thermodynamics of enols," Ch. 2 in The Chemistry of Enols, Z. Rappoport, ed. (Wiley, 1990).

DH: E. S. Domalski and E. D. Hearing, "Estimation of the Thermodynamic Properties of C-H-N-O-S-Halogen Compounds at 298.15 K," J. Phys. Chem. Ref. Data 22, 805 (1993).

P94: J. B. Pedley, "Thermochemical Data and Structures of Organic Compounds, Vol. 1 (TRC Data Series, 1994).

SWS: D. S. Stull, E. F. Westrum Jr., and G. C. Sinke, "The Chemical Thermodynamics of Organic Compounds" (Krieger, 1987).

Table 5. Carbon-Hydrogen-Oxygen compounds (CxHyO2): Enthalpy of formation (298 K), 1

Compound	Formula (PNK #)	CAS Registry No.	Gas			Liquid			Solid		
			Expt. Ref.	Calc.	Δ	Expt. Ref.	Calc.	Δ	Expt. Ref.	Calc.	Δ
Formic acid	CH2O2 (1)	64-18-6	-378.7	-375.3	-3.4	-425.1	-423.4	3.3			
Methanediol	CH4O2					-517.6 a	-450.2	-67.4			
Glyoxal (Ethanedial)	C2H2O2 (1)	107-22-2	-212.0	-210.9	-1.1						
Acetic acid	C2H4O2 (1)	64-19-7	-432.8	-431.0	-1.8	-484.3 P	-484.9	0.6			
Formic acid methyl ester	C2H4O2 (2)	107-31-3	-355.5	-355.6	0.1	-386.1	-386.2	0.1			
Ethylene glycol (1,2-Ethanediol)	C2H6O2 (1)	107-21-1	-387.5	-384.9	-2.6	-455.3	-456.9	1.6			
Ethyl hydroperoxide	C2H6O2 (2)	3031-74-1	-198.9	-164.8	-34.1	-242.0	-207.9	-34.1			
Dimethyl peroxide	C2H6O2 (3)	690-02-8	-125.7	-125.5	-0.2						
1,1-Ethanediol	C2H6O2					-498.7 b	-496.2	-2.5			
2-Propynoic acid	C3H2O2 (1)	471-25-0				-193.2	-194.1	0.9			
1,2-Propanedione (Pyruvaldehyde)	C3H4O2 (1)	78-98-8	-271.0	-273.6	2.6	-309.1	-318.0	8.9			
2-Oxetanone (beta-Propiolactone)	C3H4O2 (2)	57-57-8	-282.9	-282.8	-0.1	-329.9	-329.7	-0.2			
2-Propenoic acid (Acrylic acid)	C3H4O2 (3)	79-10-7	-322.2 S	-328.4	6.3	-383.8	-384.9	1.1			
2,3-Epoxy-1-propanol (Glycidol; hycroxymethyloxir	C3H6O2 (1)	556-52-5				-298.2	-300.4	2.2			
1,3-Dioxolane	C3H6O2 (2)	646-06-0	-298.0	-313.8	15.8	-333.5	-331.8	-1.7			
Propanoic acid	C3H6O2 (3)	79-09-4	-453.5	-452.7	-0.8	-510.7	-506.7	-4.0			
Acetic acid methyl ester	C3H6O2 (4)	79-20-9	-411.9	-411.3	-0.6	-445.8	-442.7	-3.1			
1,2-Propanediol (Propylene glycol)	C3H8O2 (1)	57-55-6	-421.3	-423.0	1.7	-485.7	-496.6	10.9			
Dimethoxymethane	C3H8O2 (2)	109-87-5	-348.4	-351.9	3.5	-377.7	-376.6	-1.1			
Propyl hydroperoxide	C3H8O2 (3)	6068-96-8				-318.0	-233.5	-84.5			
1,3-Propanediol	C3H8O2 (4)	504-63-2	-392.1	-405.8	13.7	-464.9	-482.4	17.5			
3-Butynoic acid	C4H4O2 (1)	2345-51-9							-241.8	-241.8	0.0
4-Methylene-2-oxetanone (Diketene)	C4H4O2 (2)	674-82-8	-190.2	-195.8	5.6	-233.1	-233.0	-0.1			
Cyclobutane-1,3-dione	C4H4O2 (3)	15506-53-3	-186.3	-186.2	-0.1				-260.0	-259.8	-0.2
Propynoic acid methyl ester	C4H4O2					-141.8 SWS	-151.9	10.0			
Biacetyl	C4H6O2 (1)	625-34-3	-327.1	-336.4	9.3	-365.8	-365.7	-0.1			
Acetic acid vinyl ester	C4H6O2 (2)	108-05-4	-314.9	-314.2	-0.7	-350.5 P	-346.4	-4.1			
2-Propenoic acid methyl ester	C4H6O2 (3)	96-33-3	-313.8 S	-308.8	-5.0	-362.2	-342.7	-19.5			
Tetrahydrofuran-2-one	C4H6O2 (5)	96-48-0	-366.5 P94	-368.6	2.1	-420.9 P94	-421.7	0.8			
4-Butanolactone	C4H6O2	96-48-0	-366.5 DH	-366.5	0.0	-420.9 DH	-420.9	0.0			
2-Methyl-2-propenoic acid (Methacrylic acid)	C4H6O2	79-41-4	-368.2 S	-360.7	-7.5						
2,3-Butanedione	C4H6O2	431-03-8	-327.2 CP	-336.4	9.2	-366.1 CP	-365.7	-0.4			
Butanoic acid (Butyric acid)	C4H8O2 (1)	107-92-6	-475.8	-473.6	-2.2	-533.8	-532.2	-1.6			
Acetic acid ethyl ester	C4H8O2 (2)	141-78-6	-444.1	-445.2	1.1	-479.3	-480.7	1.4			
1,4-Dioxane	C4H8O2 (3)	123-91-1	-315.8	-320.1	4.3	-353.9	-354.0	0.1			
1,3-Dioxane	C4H8O2 (4)	505-22-6	-342.3	-352.7	10.4	-379.7	-377.0	-2.7			
2-Methyl-1,3-dioxolane	C4H8O2 (5)	497-26-7	-352.0	-352.7	0.7	-386.9	-377.8	-9.1			
Formic acid propyl ester	C4H8O2 (7)	110-74-7	-462.7 c	-410.5	-52.2	-500.3	-449.8	-50.5			
1,2-Butanediol	C4H10O2 (1)	584-03-2				-523.6	-522.2	-1.4			
1,3-Butanediol	C4H10O2 (2)	107-88-0	-433.2 *	-443.9	10.7	-501.0 *	-522.2	21.2			

Table 5. Carbon-Hydrogen-Oxygen compounds (CxHyO2): Enthalpy of formation (298 K), 2

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
2,3-Butanediol	C4H10O2 (3)	513-85-9	-482.3		-461.1	-21.2	-541.5		-536.3	-5.2				
2-Methyl-1,2-propanediol	C4H10O2 (4)	558-43-0					-539.7		-539.3	-0.4				
1,1-Dimethoxyethane	C4H10O2 (5)	25154-53-4	-389.7		-390.8	1.1	-420.2		-422.6	2.4				
Diethyl peroxide	C4H10O2 (6)	628-47-5	-192.8		-193.3	0.5	-233.3		-225.1	-8.2				
tert-Butyl hydroperoxide	C4H10O2 (7)	75-91-2	-245.9		-242.2	-3.7	-293.6		-290.3	-3.3				
1,4-Butanediol	C4H10O2 (8)	110-63-4	-426.7		-426.8	0.1	-503.3		-507.9	4.6				
1,2-Dimethoxyethane	C4H10O2	110-71-4	-338.9	L	-350.6	11.7								
Furfural (2-Furaldehyde)	C5H4O2 (1)	98-01-1	-151.0		-136.4	-14.6	-201.6		-190.0	-11.6				
3-Pentynoic acid	C5H6O2 (1)	36781-65-4									-292.3		-292.5	0.2
2-Hydroxymethylfuran (Furfuryl alcohol)	C5H6O2 (2)	98-00-0	-211.8		-190.8	-21.0	-276.2		-259.0	-17.2				
2,4-Pentanedione	C5H8O2 (1)	123-54-6	-380.6		-376.6	-4.0	-423.8		-424.3	0.5				
4-Pentenoic acid	C5H8O2 (2)	591-80-0					-430.6		-431.0	0.4				
3-Pentenoic acid	C5H8O2 (3)	5204-64-8					-434.8		-442.2	7.4	-435.1	SWS	-457.7	22.6
2-Pentenoic acid	C5H8O2 (4)	626-98-2					-446.5		-447.3	0.8	-447.3	SWS	-432.6	-14.6
(E)-2-Butenoic acid methyl ester (Methyl crotonate)	C5H8O2 (5)	623-43-8	-341.9		-341.0	-0.9	-382.9		-379.5	-3.4				
Acetic acid isopropenyl ester	C5H8O2 (6)	108-22-8					-386.4		-403.3	16.9				
5-Methyltetrahydrofuran-2-one	C5H8O2 (7)		-406.5	P94	-406.7	0.2	-461.3	P94	-461.5	0.2				
Tetrahydro-2H-pyran-2-one	C5H8O2 (8)	542-28-9	-379.5	P94	-379.5	-0.0	-437.6	P94	-437.6	0.0				
4-Pentanolactone	C5H8O2	108-29-2	-406.5	DH	-406.7	0.2	-461.3	DH	-461.5	0.2				
5-Pentanolactone	C5H8O2	542-28-9	-379.6	DH	-379.5	-0.1	-437.6	DH	-437.6	0.0				
2-Methyl-2-propenoic acid methyl ester	C5H8O2	80-62-6	-347.3	L	-341.0	-6.3								
2,4-Pentanedione	C5H8O2	123-54-6	-384.9	S	-376.6	-8.4								
Acetic acid 2-propenyl ester	C5H8O2	591-87-7	-347.3	S	-336.0	-11.3								
Pentanoic acid (Valeric acid)	C5H10O2 (1)	109-52-4	-491.9		-494.5	2.6	-559.4		-557.7	-1.7				
2-Methylbutanoic acid	C5H10O2 (2)	116-53-0					-554.5		-564.8	10.3				
3-Methylbutanoic acid (Isovaleric acid)	C5H10O2 (3)	503-74-2	-510.0		-501.2	-8.8	-561.6		-562.1	0.5				
2,2-Dimethylpropanoic acid (Pivalic acid)	C5H10O2 (4)	75-98-9	-491.3		-508.8	17.5	-564.5		-567.3	2.8				
Propanoic acid ethyl ester	C5H10O2 (5)	105-37-3	-463.6		-466.9	3.3	-502.7		-502.5	-0.2				
Acetic acid isopropyl ester	C5H10O2 (6)	108-21-4	-481.7		-483.3	1.6	-518.9		-520.5	1.6				
(Z)-1,2-Cyclopentanediol	C5H10O2 (7)	5057-98-7									-485.1		-508.4	23.3
(E)-1,2-Cyclopentanediol	C5H10O2 (8)	5057-99-8									-490.1		-514.6	24.5
2-Hydroxymethyltetrahydrofuran	C5H10O2 (9)	97-99-4	-369.2		-360.2	-9.0	-435.7		-422.6	-13.1				
2,2-Dimethyl-1,3-dioxolane	C5H10O2 (10)	2916-31-6					-423.1		-425.5	2.4				
2-Methyl-1,3-dioxane	C5H10O2 (11)	626-68-6	-397.8		-391.6	-6.2	-436.4		-423.0	-13.4				
4-Methyl-1,3-dioxane	C5H10O2 (12)	1120-97-4	-376.9		-366.9	-10.0	-416.1		-388.7	-27.4				
1,3-Dioxepane	C5H10O2 (13)	505-65-7	-346.6		-346.4	-0.2	-387.6		-387.4	-0.2				
(Z)-2,4-Dimethyl-1,3-dioxolane	C5H10O2 (15)	1192-35-4	-382.6		-379.1	-3.5	-421.3		-398.3	-23.0				
(E)-2,4-Dimethyl-1,3-dioxolane	C5H10O2 (16)	1192-36-5	-380.5		-379.1	-1.4	-419.8		-398.3	-21.5				
(Ethoxymethyl)oxirane	C5H10O2 (17)	4016-11-9					-296.6	P94	-301.7	5.0				

Table 5. Carbon-Hydrogen-Oxygen compounds (CxHyO2): Enthalpy of formation (298 K), 3

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
2-Methyl-propanoic acid methyl ester	C5H10O2	547-63-1	-456.1	L	-460.2	4.2								
2,2-Dimethoxypropane (Acetone dimethyl acetal)	C5H12O2 (1)	77-76-9	-429.6		-420.9	-8.7	-459.0		-458.6	-0.4				
1,5-Pentanediol	C5H12O2 (2)	111-29-5	-449.1		-447.7	-1.4	-531.5		-533.5	2.0				
2,2-Dimethyl-',3-propanediol	C5H12O2 (3)	126-30-7	-550.4	d	-469.0	-81.3					-551.2		-551.0	-0.2
1,1-Dimethoxypropane	C5H12O2 (4)	4744-95-3					-433.3		-448.1	14.8				
Diethoxymethane (3,5-Dioxaheptane)	C5H12O2 (5)	462-95-3	-414.8		-419.7	4.9	-450.4		-452.7	2.3				
1,2-Pentanediol	C5H12O2 (6)	5343-92-0	-465.3	P94	-447.7	-17.6	-546.8	P94	-533.5	-13.4				
2,5-Cyclohexadiene-1,4-dione (p-Benzoquinone)	C6H4O2 (1)	106-51-4	-122.9		-123.0	0.1					-185.7		-185.8	0.1
1,4-Benzenediol (Hydroquinone)	C6H6O2 (1)	123-31-9	-265.3		-274.5	9.2					-364.5		-374.0	9.5
1,3-Benzenediol (Resorcinol)	C6H6O2 (2)	108-46-3	-274.7		-274.5	-0.2					-368.0		-374.0	6.0
1,2-Benzenediol (Catechol)	C6H6O2 (3)	120-80-9	-267.3	P94	-272.4	5.1					-354.1	P94	-367.8	13.7
Bicyclo[1.1.0]butane-1-carboxylic acid methyl ester	C6H8O2 (1)	4935-01-7	-164.6		-141.0	-23.6	-203.1		-195.0	-8.1				
(E)-2-Butenoic acid ethyl ester	C6H10O2 (1)	623-70-1	-375.6		-374.9	-0.7	-420.0		-417.6	-2.4				
Cyclobutanecarboxylic acid methyl ester	C6H10O2 (2)	765-85-5	-355.3		-327.2	-28.1	-395.0		-370.7	-24.3				
3-Methylpentan-2,4-dione	C6H10O2 (3)	815-57-6					-437.0	P94	-448.5	11.5				
6-Methoxy-dihydro-2H-pyran	C6H10O2		-291.3	G	-298.7	7.4								
Hexanoic acid (Caproic acid)	C6H12O2 (1)	142-62-1	-511.9		-515.5	3.6	-583.8		-583.2	-0.6				
Pentanoic acid methyl ester	C6H12O2 (2)	624-24-8	-471.2		-474.9	3.7	-514.2		-515.5	1.3				
2-Methylbutanoic acid methyl ester	C6H12O2 (3)	868-57-5	-492.5		-481.2	-11.3	-534.3		-522.6	-11.7				
3-Methylbutanoic acid methyl ester	C6H12O2 (4)	556-24-1	-497.9		-484.9	-13.0	-538.9		-522.2	-16.7				
2,2-Dimethylpropanoic acid methyl ester	C6H12O2 (5)	598-98-1	-494.3		-489.1	-5.2	-530.0		-525.1	-4.9				
Acetic acid butyl ester	C6H12O2 (6)	123-86-4	-485.6		-487.0	1.4	-529.2		-531.8	2.6				
Cyclohexyl hydroperoxide	C6H12O2 (7)	766-07-4					-273.2		-281.2	8.0				
Tetrahydro-2-methoxy-pyran	C6H12O2 (8)	6581-66-4	-399.6		-399.2	-0.4	-442.2		-441.4	-0.8				
(Z)-2,4-Dimethyl-1,3-dioxane	C6H12O2 (9)	15042-59-8	-425.3		-429.7	4.4	-465.2		-462.8	-2.4				
4,5-Dimethyl-1,3-dioxane	C6H12O2 (10)	15042-60-1	-409.1		-418.4	9.3	-451.6		-446.6	-5.0				
5,5-Dimethyl-1,3-dioxane	C6H12O2 (11)	872-98-0	-420.1		-415.9	-4.2	-461.3		-445.2	-16.1				
1,3-Dioxocane	C6H12O2 (12)	6572-90-3	-336.8		-336.8	0.0	-378.7		-378.7	-0.0				
(Z)-4,6-Dimethyl-1,3-dioxane	C6H12O2 (13)	3390-18-9					-474.8		-456.5	-18.3				
(E)-4,6-Dimethyl-1,3-dioxane	C6H12O2 (14)	1121-87-5					-462.6		-451.9	-10.7				
2,2-Dimethyl-1,3-dioxane	C6H12O2 (15)	695-30-7					-468.9		-445.2	-23.7				
(Propoxymethyl)oxirane	C6H12O2 (17)	3126-95-2	-272.6	P94	-280.7	8.1	-319.9		-327.2	7.3				
(Isopropoxymethyl)oxirane	C6H12O2 (18)	4016-14-2	-298.7	P94	-301.7	2.9	-343.1	P94	-350.2	7.1				
Acetic acid 1-methylpropyl ester	C6H12O2	105-46-4	-502.1	L	-504.2	2.1								
2,4-Dimethyl-1,3-dioxane	C6H12O2	766-20-1	-426.8	S	-433.9	7.1								
3,3,4,4-Tetramethyl-1,2-dioxetane	C6H12O2	35856-82-7	-171.6	S	-175.7	4.1								
(Z)-1-Methyl-1,2-cyclopentanediol	C6H12O2										-529.7	SWS	-563.6	33.9
(E)-1-Methyl-1,2-cyclopentanediol	C6H12O2										-539.3	SWS	-563.6	24.3
(Z)-1,2-Cyclohexanediol	C6H12O2	1792-81-0									-555.2	SWS	-538.9	-16.3

Table 5. Carbon-Hydrogen-Oxygen compounds (CxHyO2): Enthalpy of formation (298 K), 4

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
(E)-1,2-Cyclohexanediol	C6H12O2	931-17-9									-551.0	SWS	-542.2	-8.8
Propanoic acid propyl ester	C6H12O2						-533.0	SWS	-528.0	-5.0				
4-Hydroxy-4-methyl-2-pentanone	C6H12O2	123-42-2					-530.5	SWS	-532.6	2.1				
Hexyl hydroperoxide	C6H14O2 (1)	4312-76-9					-299.6		-310.0	10.4				
1-Methylpentyl hydroperoxide	C6H14O2 (2)	24254-55-5					-310.1		-322.0	11.9				
1-Ethylbutyl hydroperoxide	C6H14O2 (3)	24254-56-6					-305.1		-319.7	14.6				
1,6-Hexanediol	C6H14O2 (4)	629-11-8	-461.2		-468.6	7.4	-544.4		-559.0	14.6	-569.9		-577.4	7.5
1,2-Diethoxyethane	C6H14O2 (5)	629-14-1	-408.2		-418.4	10.2	-451.4		-459.4	8.0				
2,2-Dimethoxybutane	C6H14O2 (6)	3453-99-4					-485.1		-473.6	-11.5				
1,1-Diethoxyethane	C6H14O2 (7)	105-57-7	-453.5		-458.6	5.1	-491.4		-498.7	7.3				
1,1-Dimethoxybutane	C6H14O2 (8)	4461-87-4					-468.1		-473.6	5.5				
1,1-Dimethoxy-2-methylpropane	C6H14O2 (9)	41632-89-7					-476.2		-480.3	4.1				
1,2-Hexanediol	C6H14O2 (18)	6920-22-5	-489.9	P94	-468.6	-21.3	-577.0	P94	-559.0	-18.0				
bis(1-Methylethyl) peroxide	C6H14O2	16642-57-2	-272.0	S	-269.4	-2.5								
Benzoic acid	C7H6O2 (1)	65-85-0	-294.1		-301.2	7.1	-372.8	D	-372.8	-0.0	-385.2		-377.4	-7.8
Methylenedioxybenzene (1,3-Benzodioxole)	C7H6O2 (2)	274-09-9	-142.7		-142.3	-0.4	-184.1		-183.9	-0.2				
2-Hydroxy-2,4,6-cycloheptatriene-1-one	C7H6O2 (3)	533-75-5	-155.4		-145.2	-10.2					-239.3		-246.4	7.1
Formic acid phenyl ester	C7H6O2 (4)	1864-94-4	-215.8		-221.8	6.0	-268.7		-271.1	2.4				
3-(2-Furyl)-2-propenal	C7H6O2 (5)	623-30-3	-105.9		-95.0	-10.9					-182.0		-182.0	-0.0
3-Methyl-1,2-benzenediol	C7H8O2 (1)		-299.3	P94	-302.9	3.6					-392.5	P94	-397.9	5.4
4-Methyl-1,2-benzenediol	C7H8O2 (2)		-298.3	P94	-305.0	6.7					-393.3	P94	-404.2	10.9
2-Hexynoic acid methyl ester	C7H10O2 (1)	18937-79-6					-242.7		-250.2	7.5				
4-Pentynoic acid ethyl ester	C7H10O2 (2)	63093-41-4	-233.2		-216.7	-16.5	-281.7		-260.7	-21.0				
3-Pentynoic acid ethyl ester	C7H10O2 (3)	52750-56-8	-237.8		-237.7	-0.1	-287.6		-287.9	0.3				
2-Pentynoic acid ethyl ester	C7H10O2 (4)	55314-57-3	-250.3		-249.8	-0.5	-301.8		-262.8	-39.0				
2-Methylene-3-butenoic acid ethyl ester	C7H10O2 (5)	44804-88-8	-289.7		-274.9	-14.8	-338.2		-338.5	0.3				
1-(2-Furyl)propan-1-ol	C7H10O2 (6)	26908-23-6					-447.0		-455.2	8.2				
Ethyl 2,4-pentadienoate	C7H10O2	13038-12-5	-289.7	CP	-298.3	8.6	-338.2	CP	-359.0	20.8				
4-Pentenoic acid ethyl ester	C7H12O2 (1)	1968-40-7	-385.6		-382.8	-2.8	-431.6		-426.8	-4.8				
(Z)-3-Pentenoic acid ethyl ester	C7H12O2 (2)	27829-70-5	-387.6		-390.4	2.8	-432.4		-434.3	1.9				
(E)-3-Pentenoic acid ethyl ester	C7H12O2 (3)	3724-66-1	-390.2		-395.0	4.8	-437.0		-438.1	1.1				
(Z)-2-Pentenoic acid ethyl ester	C7H12O2 (4)	27805-84-1	-394.8		-402.9	8.1	-440.8		-461.9	21.1				
(E)-2-Pentenoic acid ethyl ester	C7H12O2 (5)	24410-84-1	-394.3		-407.5	13.2	-442.5		-465.7	23.2				
(E)-2-Butenoic acid propyl ester	C7H12O2 (6)	10352-87-1	-395.2		-395.8	0.6	-443.3		-443.1	-0.2				
(E)-2-Butenoic acid isopropyl ester	C7H12O2 (7)	18060-77-0	-411.1		-413.0	1.9	-451.7		-457.3	5.6				
Heptanoic acid	C7H14O2 (1)	111-14-8	-536.2		-536.4	0.2	-610.2		-608.8	-1.4				
Hexanoic acid methyl ester	C7H14O2 (2)	106-70-7	-492.6		-495.8	3.2	-540.2		-541.0	0.8				
Pentanoic acid ethyl ester	C7H14O2 (3)	539-82-2	-506.9		-495.8	-11.1	-553.0		-541.0	-12.0				
2-Methylbutanoic acid ethyl ester	C7H14O2 (4)	7452-79-1	-522.4		-515.1	-7.3	-566.8		-560.7	-6.1				
3-Methylbutanoic acid ethyl ester	C7H14O2 (5)	108-64-5	-527.0		-518.8	-8.2	-570.9		-560.2	-10.7				

Table 5. Carbon-Hydrogen-Oxygen compounds (CxHyO2): Enthalpy of formation (298 K), 5

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
2,2-Dimethylpropanoic acid ethyl ester	C7H14O2 (6)	3938-95-2	-536.0		-523.0	-13.0	-577.2		-563.2	-14.0				
(2a,4a,6a)-2,4,6-Trimethyl-1,3-dioxane	C7H14O2 (7)	19145-91-6	-445.1		-454.4	9.3	-488.2		-492.0	3.8				
1-Methylcyclohexyl hydroperoxide	C7H14O2 (8)	4952-03-8					-330.4		-313.4	-17.0				
2,2,4-Trimethyl-1,3-dioxane	C7H14O2 (9)	696-79-7	-460.7	e	-463.2	2.5	-502.5	e	-502.3	-0.2				
4,4,6-Trimethyl-1,3-dioxane	C7H14O2 (10)	1123-07-5					-500.5		-499.2	-1.3				
(tert-Butoxymethyl)oxirane	C7H14O2 (12)	7665-72-7					-370.1		-380.3	10.2				
(Butoxymethyl)oxirane	C7H14O2 (13)	2426-08-6	-292.0	P94	-297.9	5.9	-345.2	P94	-343.9	-1.3				
(2-Methylpropoxymethyl)oxirane	C7H14O2 (14)	3814-55-9	-306.7	P94	-311.7	5.0	-357.7	P94	-359.4	1.7				
(Z)-1-Methyl-1,2-cyclohexanediol	C7H14O2										-603.3	SWS	-605.2	1.9
(E)-1-Methy-1,2-cyclohexanediol	C7H14O2										-593.3	SWS	-605.2	11.9
2,2-Diethoxypropane (Acetone diethyl acetal)	C7H16O2 (1)	126-84-1	-506.6		-488.7	-17.9	-538.5		-534.7	-3.8				
1-Heptyl hydroperoxide	C7H16O2 (2)	764-81-8					-343.0		-335.6	-7.4				
2-Heptyl hydroperoxide	C7H16O2 (3)						-346.4		-349.8	3.4				
3-Heptyl hydroperoxide	C7H16O2 (4)						-346.8		-349.8	3.0				
4-Heptyl hydroperoxide	C7H16O2 (5)						-333.8		-349.8	16.0				
2,2-Dimethoxypentane	C7H16O2 (6)	55304-08-4					-509.2		-509.6	0.4				
2,2-Dimethoxy-3-methyl-butane	C7H16O2 (7)	59554-08-4					-512.2		-514.0	1.8				
1,3-Diethoxypropane	C7H16O2 (8)	3459-83-4	-436.2		-439.3	3.1	-482.1		-484.9	2.8				
1,1-Dimethoxypentane	C7H16O2 (9)	26450-58-8					-494.6		-517.6	23.0				
1,7-Heptanediol	C7H16O2 (12)	629-30-1					-574.0	P94	-584.5	10.5				
2-Methoxybenzaldehyde (Anisaldehyde)	C8H8O2 (1)	135-02-4									-266.4		-259.4	-7.0
3-Methoxybenzaldehyde	C8H8O2 (2)	591-31-1					-276.0		-255.1	-20.9				
4-Methoxybenzaldehyde	C8H8O2 (3)	123-11-5	-202.7		-187.0	-15.7	-267.2		-255.1	-12.1				
1-(2-Hydroxyphenyl)ethanone	C8H8O2 (4)	118-93-4									-357.6		-360.7	3.1
1-(3-Hydroxyphenyl)ethanone	C8H8O2 (5)	121-71-1									-370.6		-363.2	-7.4
1-(4-Hydroxyphenyl)ethanone	C8H8O2 (6)	99-93-4									-364.3		-363.2	-1.1
2-Methylbenzoic acid (o-Toluic acid)	C8H8O2 (7)	118-90-1	-320.1	S	-321.3	1.3					-416.5		-409.6	-6.9
3-Methylbenzoic acid	C8H8O2 (8)	99-04-7	-329.7	S	-333.9	4.2					-426.1		-413.8	-12.3
4-Methylbenzoic acid	C8H8O2 (9)	99-94-5	-332.2	S	-333.9	1.7					-429.2		-413.8	-15.4
Acetic acid phenyl ester	C8H8O2 (10)	122-79-2	-279.7		-277.4	-2.3	-334.9		-327.6	-7.3				
2,3-Dihydro-1,4-benzodioxin	C8H8O2 (11)	493-09-4	-204.1		-203.8	-0.3	-254.7		-254.6	-0.1				
Benzoic acid methyl ester	C8H8O2 (12)	93-58-3	-287.9		-281.6	-6.3	-343.5		-330.5	-13.0				
4-(2-Furyl)-3-buten-2-one	C8H8O2 (13)	623-15-4									-240.2		-233.8	-6.4
1,2-Dimethoxybenzene	C8H10O2 (1)	91-16-7	-223.3		-204.2	-19.1	-290.3		-285.2	-5.1				
1,4-Benzenedimethanol	C8H10O2 (2)	589-29-7									-393.9		-394.1	0.2
2,2,4,4-Tetramethyl-1,3-cyclobutanedione	C8H12O2 (3)	933-52-8	-307.6		-307.1	-0.5					-379.9		-379.1	-0.8
1-(3,4-Dihycro-6-methyl-2H-pyran-2-yl) ethanone	C8H12O2	28450-02-4	-330.5	S	-330.5									
(E)-2-Butenoic acid butyl ester	C8H14O2 (1)	7299-91-4	-415.9		-416.7	0.8	-467.8		-468.6	0.8				
(E)-2-Butenoic acid tert-butyl ester	C8H14O2 (2)	3246-27-3	-423.9		-452.3	28.4	-474.1		-500.0	25.9				

Table 5. Carbon-Hydrogen-Oxygen compounds (CxHyO2): Enthalpy of formation (298 K), 6

Compound	Formula (PNK #)	CAS Registry No.	Gas			Liquid			Solid		
			Expt. Ref.	Calc.	Δ	Expt. Ref.	Calc.	Δ	Expt. Ref.	Calc.	Δ
(E)-2-Butenoic acid 1-methylpropyl ester	C8H14O2 (3)	10371-45-6	-425.1	-433.9	8.8	-474.5	-482.8	8.3			
4-Pentenoic acid propyl ester	C8H14O2 (4)	62030-43-7	-397.9	-391.2	-6.7	-447.3	-429.7	-17.6			
4-Pentenoic acid isopropyl ester	C8H14O2 (5)	62030-44-8	-417.2	-408.4	-8.8	-464.5	-443.9	-20.6			
3-Pentenoic acid propyl ester	C8H14O2 (6)	62030-40-4	-404.2	-393.7	-10.5	-454.4	-443.9	-10.5			
3-Pentenoic acid isopropyl ester	C8H14O2 (7)	62030-41-5	-425.1	-414.6	-10.5	-473.3	-466.9	-6.4			
2-Pentenoic acid propyl ester	C8H14O2 (8)	62030-39-1	-413.0	-412.1	-0.9	-464.9	-459.8	-5.1			
2-Pentenoic acid isopropyl ester	C8H14O2 (9)		-429.3	-433.0	3.7	-478.7	-482.8	4.1			
2-Methylene-3,3-dimethylbutanoic acid methyl ester	C8H14O2 (10)	79593-50-3				-421.4	-434.5	13.1			
1-(2-Hydroxycyclopentyl)-2-proparone	C8H14O2 (11)					-472.0	-504.6	32.6			
2,5-Dimethyl-3-hexyne-2,5-diol	C8H14O2 (12)	142-30-3							-385.7	-374.9	-10.8
2-Ethoxy-3,4-dihydro-6-methyl-2H-pyran	C8H14O2	52438-71-8	-472.8 S	-373.2	-99.6						
Octanoic acid (Caprylic acid)	C8H16O2 (1)	124-07-2	-554.3	-557.3	3.0	-636.0	-634.3	-1.7			
Heptanoic acid methyl ester	C8H16O2 (2)	106-73-0	-515.9	-516.7	0.8	-567.1	-566.5	-0.6			
Pentanoic acid propyl ester	C8H16O2 (3)	141-06-0	-533.6	-529.7	-3.9	-583.0	-579.1	-3.9			
Pentanoic acid isopropyl ester	C8H16O2 (4)	18362-97-5	-544.9	-546.8	1.9	-592.2	-593.3	1.1			
Butanoic acid 1-methylpropyl ester	C8H16O2 (5)	819-97-6	-545.3	-546.8	1.5	-592.6	-593.3	0.7			
2,3,3-Trimethylbutanoic acid methyl ester	C8H16O2 (6)	19910-30-6				-506.4	-579.3	72.9			
(Z)-2,2,4,6-Tetramethyl-1,3-dioxane	C8H16O2 (7)	17227-17-7	-485.3 e	-497.9	12.6	-539.4	-539.7	0.3			
(E)-2,2,4,6-Tetramethyl-1,3-dioxane	C8H16O2 (8)	20268-00-2	-498.3 d	-491.2	-7.1	-526.3	-533.9	7.6			
((1,1-Dimethylpropoxy)-methyl)oxirane	C8H16O2 (10)	42426-06-2	-337.5 P94	-348.1	10.6	-392.6	-401.5	8.9			
(Pentyloxymethyl)oxirane	C8H16O2 (11)	7297-11-2				-367.4	-378.2	10.8			
2-Ethylhexanoic acid	C8H16O2 (12)	149-57-5	-559.5	-563.6	4.1	-635.1	-641.4	6.3			
((3-Methylbutoxy)methyl)oxirane	C8H16O2 (13)	45832-22-2	-328.2 P94	-332.6	4.4	-384.0 P94	-384.9	0.9			
((2,2-Dimethylpropoxy)methyl)oxirane	C8H16O2 (14)	78906-14-6	-319.4 P94	-337.2	17.8	-369.9 P94	-389.5	19.6			
Di-tert-butylperoxide	C8H18O2 (1)	110-05-4	-349.1	-348.1	-1.0	-380.9	-389.8	8.9			
1,1-Bis(1-methylethoxy)ethane	C8H18O2 (2)		-526.1	-534.7	8.6	-569.2	-578.2	9.0			
2,5-Dimethyl-1,5-hexanediol	C8H18O2 (3)	110-03-2							-681.7	-664.8	-16.9
2,2-Dimethoxy-3,3-dimethylbutane	C8H18O2 (4)	62038-48-6				-524.4	-545.6	21.2			
1,8-Octanediol	C8H18O2 (7)	629-41-4							-626.8 P94	-636.0	9.2
2,4,6-Trimethyl-3,5-dioxaheptane	C8H18O2		-525.9 f	-521.3	-4.6	-544.3 f	-566.5	22.2			
(Z)-3-Phenyl-2-propenoic acid	C9H8O2 (1)	102-94-3							-312.1	-322.6	10.5
(E)-3-Phenyl-2-propenoic acid (Cinnamic acid)	C9H8O2 (2)	140-10-3							-336.9	-326.8	-10.1
2,3-Dimethylbenzoic acid	C9H10O2 (1)	603-79-2	-345.8 P	-351.5	5.7				-450.4	-443.5	-6.9
2,4-Dimethylbenzoic acid	C9H10O2 (2)	611-01-8	-355.0 P	-354.0	-1.0				-458.5	-446.0	-12.5
2,5-Dimethylbenzoic acid	C9H10O2 (3)	610-72-0	-351.1 P	-354.0	2.9				-456.1	-446.0	-10.1
2,6-Dimethylbenzoic acid	C9H10O2 (4)	632-46-2	-341.4 S	-341.4					-440.7	-441.8	1.1
3,4-Dimethylbenzoic acid	C9H10O2 (5)	619-04-5	-362.4 P	-364.0	1.6				-468.8	-447.7	-21.1
3,5-Dimethylbenzoic acid	C9H10O2 (6)	499-06-9	-364.5 P	-366.5	2.0				-466.4	-450.2	-16.2
Acetic acid 3-methylphenyl ester	C9H10O2 (7)	122-46-3	-313.4	-310.0	-3.4	-374.1	-364.3	-9.8			

Table 5. Carbon-Hydrogen-Oxygen compounds (CxHyO2): Enthalpy of formation (298 K), 7

Compound	Formula (PNK #)	CAS Registry No.	Gas			Liquid			Solid		
			Expt. Ref.	Calc.	Δ	Expt. Ref.	Calc.	Δ	Expt. Ref.	Calc.	Δ
3,4-Dihydro-2H-1,5-benzodioxepin	C9H10O2 (8)	7216-18-4	-185.5	-185.4	-0.1	-241.1	-241.2	0.1			
2-Ethylbenzoic acid	C9H10O2 (9)	612-19-1	-340.6	-340.6	-0.0				-441.3	-436.8	-4.5
3-Ethylbenzoic acid	C9H10O2 (10)	619-20-5	-346.7	-353.1	6.4				-445.8	-441.0	-4.8
4-Ethylbenzoic acid	C9H10O2 (11)	619-64-7	-363.2	-353.1	-10.1				-460.7	-441.0	-19.7
(Z)-1,2-Indandiol	C9H10O2								-373.2 SWS	-385.8	12.6
(E)-1,2-Indandiol	C9H10O2								-380.7 SWS	-388.3	7.5
1-Methyl-1-phenylethylhydroperoxide	C9H12O2 (1)	80-15-9	-78.4	-98.3	19.9	-148.3	-149.8	1.5	-161.8 DH	-112.3	-49.5
3-Isopropyl-1,2-benzenediol	C9H12O2 (2)	2138-48-9	-350.0 P94	-348.9	-1.1				-447.8 P94	-444.3	-3.5
(E)-2-Butenoic acid 3-methylbutyl ester	C9H16O2 (1)	25415-77-4	-446.8	-444.3	-2.5	-500.7	-498.5	-2.2			
4-Pentenoic acid butyl ester	C9H16O2 (2)	22874-80-2	-427.1	-424.7	-2.4	-479.8	-477.8	-2.0			
4-Pentenoic acid 2-methylpropyl ester	C9H16O2 (3)		-436.7	-444.8	8.1	-488.2	-493.7	5.5			
4-Pentenoic acid 1-methylpropyl ester	C9H16O2 (4)		-446.3	-441.8	-4.5	-497.0	-492.0	-5.0			
3-Pentenoic acid butyl ester	C9H16O2 (5)	19825-93-5	-433.0	-431.0	-2.0	-486.5	-500.8	14.3			
3-Pentenoic acid 2-methylpropyl ester	C9H16O2 (6)		-453.0	-448.1	-4.9	-505.3	-515.1	9.8			
3-Pentenoic acid 1-methylpropyl ester	C9H16O2 (7)		-451.4	-448.1	-3.3	-502.8	-515.1	12.3			
2-Pentenoic acid butyl ester	C9H16O2 (8)		-439.7	-449.4	9.7	-494.9	-516.7	21.8			
2-Pentenoic acid 2-methylpropyl ester	C9H16O2 (9)		-453.0	-459.4	6.4	-506.6	-523.4	16.8			
2-Pentenoic acid 1-methylpropyl ester	C9H16O2 (10)		-457.6	-466.5	8.9	-510.4	-530.9	20.5			
3-Hydroxy-2,2-dimethyl-3-hepten-5-one	C9H16O2		-470.7 g	-464.4	-6.3	-527.8 g	-528.0	0.2			
3-Hydroxy-2,6-dimethyl-3-hepten-5-one	C9H16O2		-470.3 g	-464.8	-5.4	-527.3 g	-524.3	-3.0			
2,2-Dimethylheptane-3,5-dione	C9H16O2		-470.2 c	-476.1	5.9	-527.1 g	-528.4	1.3			
2,6-Dimethylheptane-3,5-dione	C9H16O2		-470.7 c	-474.5	3.7	-526.8 g	-533.0	6.2			
Nonanoic acid	C9H18O2 (1)	112-05-0	-577.3	-578.2	0.9	-659.7	-659.8	0.1			
Octanoic acid methyl ester	C9H18O2 (2)	111-11-5	-533.8	-537.6	3.8	-590.3	-592.0	1.7			
Pentanoic acid butyl ester	C9H18O2 (3)	591-68-4	-560.2	-550.6	-9.6	-613.3	-604.6	-8.7			
Pentanoic acid 2-methylpropyl ester	C9H18O2 (4)	10588-10-0	-568.6	-560.7	-7.9	-620.0	-611.3	-8.7			
Pentanoic acid 1-methylpropyl ester	C9H18O2 (5)	23361-74-2	-573.2	-567.8	-5.4	-624.2	-618.8	-5.4			
Dibutoxymethane	C9H20O2 (1)	2568-90-3	-501.3	-503.3	2.0	-549.4	-554.8	5.4			
2,6-Dimethyl-2,6-heptanediol	C9H20O2 (2)	6257-51-8							-761.1	-715.5	-45.6
1,9-Nonanediol	C9H20O2 (4)	3937-56-2							-657.7 P94	-665.3	7.5
1,4-Naphthalenedione (1,4-Naphthoquinone)	C10H6O2 (1)	130-15-4	-111.0	-125.9	14.9				-183.4	-183.7	0.3
2,7-Dihydroxynaphthalene (2,7-Naphthalenediol)	C10H8O2 (1)	582-17-2							-326.1	-326.4	0.3
2,3-Dihydroxynaphthalene	C10H8O2 (2)	92-44-4	-192.8 i	-205.0	12.2				-316.4	-323.8	7.4
1,2-Dihydroxynaphthalene	C10H8O2 (3)	574-00-4	-200.5 i	-205.0	4.5				-309.8 DH	-323.8	14.0
1,3-Dihydroxynaphthalene	C10H8O2 (4)	132-86-5	-211.2 i	-207.5	-3.7				-327.2 DH	-326.4	-0.8
1,4-Dihydroxynaphthalene	C10H8O2 (5)	571-60-8	-197.0 i	-207.5	10.5				-317.4 DH	-326.4	9.0
(Z)-2-Phenylcyclopropane-carboxylic acid	C10H10O2 (1)	939-89-9				-320.7	-297.9	-22.8			
(E)-2-Phenylcyclopropane-carboxylic acid	C10H10O2 (2)	939-90-2				-332.2	-297.9	-34.3			
(E)-3-(2-Methylphenyl)-2-propenoic acid	C10H10O2	939-57-1	-272.0 S	-265.7	-6.3						
Benzoylacetone	C10H10O2		-251.3 g	-246.9	-4.4				-335.1 g	-338.9	3.8

Table 5. Carbon-Hydrogen-Oxygen compounds (CxHyO2): Enthalpy of formation (298 K), 8

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
2,4-Dimethylbenzeneacetic acid	C10H12O2 (1)										-495.8		-444.8	-51.0
2,3,4-Trimethylbenzoic acid	C10H12O2 (2)	1076-47-7	-377.5	P	-381.6	4.1					-486.6		-477.4	-9.2
2,3,5-Trimethylbenzoic acid	C10H12O2 (3)	2437-66-3	-382.2	P	-384.1	1.9					-488.7		-479.9	-8.8
2,3,6-Trimethylbenzoic acid	C10H12O2 (4)	2529-36-4	-371.4	P	-384.1	12.7					-475.7		-479.9	4.2
2,4,5-Trimethylbenzoic acid	C10H12O2 (5)	528-90-5	-386.2	P	-384.1	-2.1					-495.7		-479.9	-15.8
2,4,6-Trimethylbenzoic acid	C10H12O2 (6)	480-63-7	-374.4	P	-386.6	12.2					-477.9		-482.4	4.5
3,4,5-Trimethylbenzoic acid	C10H12O2 (7)	1076-88-6	-390.1	P	-394.1	4.0					-500.9		-481.6	-19.3
2-Hydroxy-4-isopropyl-2,4,6-cycloheptatrien--1-one	C10H12O2 (8)	499-44-5									-340.6		-333.0	-7.6
1,2,3,4-Tetrahydro-5-hydroperoxynaphthalene	C10H12O2 (9)	26447-24-5									-185.7		-198.9	13.2
1,2-Epoxy-4-oxa-5-phenylpentane	C10H12O2 (13)		-138.1	P94	-143.9	5.9	-209.2	P94	-154.0	-55.2				
2-Isopropylbenzoic acid (o-cuminic acid)	C10H12O2 (10)	2438-04-2	-359.2	P	-367.4	8.2					-460.2	P	-456.1	-4.1
3-Isopropylbenzoic acid (m-cuminic acid)	C10H12O2 (11)	5651-47-8	-375.5	P	-379.9	4.4					-479.6	P	-460.2	-19.4
4-Isopropylbenzoic acid (cumic acid)	C10H12O2 (12)	536-66-3	-382.7	P	-379.9	-2.8					-483.8	P	-460.2	-23.6
(Z)-1,2,3,4-Tetrahydronaphthalene-2,3-diol	C10H12O2										-415.5	SWS	-440.1	24.6
(E)-1,2,3,4-Tetrahydronaphthalene-2,3-diol	C10H12O2										-420.9	SWS	-440.2	19.2
(Z)-1,2,3,4-Tetrahydronaphthalene-1,2-diol	C10H12O2										-415.5	SWS	-437.6	22.1
(E)-1,2,3,4-Tetrahydronaphthalene-1,2-diol	C10H12O2										-420.9	SWS	-437.6	16.7
4-tert-Butyl-1,2-benzenediol	C10H14O2 (1)		-374.7	P94	-376.6	1.9					-474.0	P94	-487.0	13.0
3-Methyl-6-isopropyl-1,2-benzenediol	C10H14O2 (2)		-379.1	P94	-379.5	0.4					-475.7	P94	-474.5	-1.2
(E)-4a-hydroperoxy-decahydronaphthalene	C10H18O2 (1)										-349.2		-419.0	69.8
2,2,6-Trimethyl-3-hydroxy-3-hepten-5-one	C10H18O2		-510.9	g	-492.0	-18.8	-568.4	c	-556.9	-11.5				
2,2,6-Trimethylheptane-3,5-dione	C10H18O2		-510.4	c	-496.2	-14.1	-568.1	c	-555.2	-12.9				
Decanoic acid (Capric acid)	C10H20O2 (1)	334-48-5	-594.9		-599.1	4.2	-684.3		-685.3	1.0	-713.7		-713.8	0.1
Nonanoic acid methyl ester	C10H20O2 (2)	1731-84-6	-553.9		-558.6	4.7	-616.2		-617.6	1.4				
((1,1-Dimethylpentyloxy)-methyl)oxirane	C10H20O2 (3)	42426-07-3					-442.1		-452.5	10.4				
1,10-Decanediol	C10H22O2 (1)	112-47-0									-693.5		-694.5	1.0
2,7-Dimethyl-2,7-octanediol	C10H22O2 (2)	19781-07-8									-730.0		-744.8	14.8
1-Naphthalenecarboxylic acid	C11H8O2 (1)	86-55-5	-223.1		-234.3	11.2					-333.5		-329.7	-3.8
2-Naphthalenecarboxylic acid	C11H8O2 (2)	93-09-4	-232.5		-234.3	1.8					-346.1		-329.7	-16.4
1,4,4a,8a-Tetrahydro-1,4-methanonaphthalene-5,8-dione	C11H10O2 (1)	1200-89-1									-164.2		-164.0	-0.2
4-(2-Methoxyphenyl)but-3-en-2-one	C11H10O2	10542-87-7	-179.9	S	-183.7	3.8								
2,3,4,5-Tetramethylbenzoic acid	C11H14O2 (1)	2529-39-7	-398.7	h	-425.5	26.8					-514.4		-517.6	3.2
2,3,4,6-Tetramethylbenzoic acid	C11H14O2 (2)	2408-38-0	-398.1	h	-428.0	29.9					-507.7		-520.1	12.4
2,3,5,6-Tetramethylbenzoic acid	C11H14O2 (3)	2604-45-7	-400.1	h	-428.0	27.9					-506.1		-520.1	14.0
1,2,3,4-Tetrahydro-1-methylhydroperoxy-naphthalene	C11H14O2 (4)										-157.2		-213.6	56.4
3,5-Diethylbenzoic acid	C11H14O2 (5)	3854-90-8	-407.8		-405.0	-2.8					-511.9		-504.6	-7.3
2-tert-Butylbenzoic acid	C11H14O2 (6)	1077-58-3	-376.1		-376.1	0.0					-476.2		-475.3	-0.9
3-tert-Butylbenzoic acid	C11H14O2 (7)	7498-54-3	-400.8		-405.4	4.6					-504.3		-496.6	-7.7

Table 5. Carbon-Hydrogen-Oxygen compounds (CxHyO2): Enthalpy of formation (298 K), 9

Compound	Formula (PNK #)	CAS Registry No.	Gas			Liquid			Solid		
			Expt. Ref.	Calc.	Δ	Expt. Ref.	Calc.	Δ	Expt. Ref.	Calc.	Δ
4-tert-Butylbenzoic acid	C11H14O2 (8)	98-73-4	-398.5	-405.4	6.9				-502.9	-496.6	-6.3
Adamantane-1-carboxylic acid	C11H16O2 (1)	828-51-3							-643.1 P94	-604.2	-38.9
Adamantane-2-carboxylic acid	C11H16O2 (2)	15897-81-1							-627.2 P94	-607.5	-19.7
2,2,6,6-Tetramethyl-3,5-heptanedione	C11H20O2	1118-71-4	-527.2 S	-532.2	5.0	-587.7 c	-589.1	1.4			
2,2,6,6-Tetramethyl-3-hydroxy-hept-3-ene-5-one	C11H20O2		-528.4 h	-520.9	-7.5	-587.9 c	-584.9	-3.0			
Undecanoic acid	C11H22O2 (1)	112-37-8	-614.6	-620.1	5.5	-710.2 D	-710.9	0.7	-735.9	-743.1	7.2
Decanoic acid methyl ester	C11H22O2 (2)	110-42-9	-573.8	-579.5	5.7	-640.5	-643.1	2.6			
1,1-Dibutoxypropane	C11H24O2 (1)	13002-10-3	-552.7	-563.2	10.5	-608.6	-626.3	17.7			
6-Ethyl-5,7-dioxaundecane	C11H24O2		-552.7 f	-563.2	10.5	-608.8 f	-626.3	17.6			
1-Acetoxynaphthalene	C12H10O2 (1)	830-81-9							-305.0	-262.3	-42.7
2-Acetoxynaphthalene	C12H10O2 (2)	1523-11-1							-309.6	-262.3	-47.3
1-Naphthaleneacetic acid	C12H10O2 (3)	86-87-3							-359.2	-326.8	-32.4
2-Naphthaleneacetic acid	C12H10O2 (4)	581-96-4							-371.9	-326.8	-45.1
Pentamethylbenzoic acid	C12H16O2 (1)	2243-32-5	-422.9 h	-429.3	6.4				-536.1	-541.0	4.9
(Z)-1-Phenyl-1,2-cyclohexanediol	C12H16O2								-467.8 SWS	-436.8	-31.0
(E)-1-Phenyl-1,2-cyclohexanediol	C12H16O2								-464.0 SWS	-436.8	-27.2
Adamantane-1-carboxylic acid methyl ester	C12H18O2 (1)	711-01-3	-495.4 P94	-488.3	-7.1				-577.8 P94	-573.6	-4.2
3,6-Diethyloct-4-yne-3,6-diol	C12H22O2 (1)	2044-37-3							-481.5	-492.0	10.5
Dodecanoic acid (Lauric acid)	C12H24O2 (1)	143-07-7	-642.0	-641.0	-1.0	-737.9	-736.4	-1.5	-774.6	-772.4	-2.2
Undecanoic acid methyl ester	C12H24O2 (2)	1731-86-8	-593.8	-600.4	6.6	-665.2	-668.6	3.4			
Octanoic acid tert-butyl ester	C12H24O2 (3)	5457-66-9				-698.7	-712.5	13.8			
2,9-Dimethyl-2,9-decanediol	C12H26O2 (1)	22092-57-5							-789.6	-803.3	13.7
Xanthone (Xanthen-9-one)	C13H8O2 (1)	90-47-1	-83.7 S	-82.8	-0.8				-191.5	-191.6	0.1
Benzoic acid phenyl ester	C13H10O2 (1)	93-99-2	-142.6	-147.7	5.1				-241.6	-239.7	-1.9
Biphenyl-2-carboxylic acid	C13H10O2 (2)	947-84-2							-349.1	-323.4	-25.7
Tridecanoic acid	C13H26O2 (1)	638-53-9	-660.2	-661.9	1.7	-763.5	-761.9	-1.6	-806.6	-801.7	-4.9
Dodecanoic acid methyl ester	C13H26O2 (2)	111-82-0	-614.8	-621.3	6.5	-693.0	-694.1	1.1			
2,10-Dimethyl-2,10-undecanediol	C13H28O2 (1)	22092-58-6							-835.8	-832.6	-3.2
9,10-Anthracenedione (Anthraquinone)	C14H8O2 (1)	84-65-1	-95.4	-94.6	-0.8				-188.5	-207.5	19.0
9,10-Phenanthrenedione	C14H8O2 (2)	84-11-7	-139.2	-138.9	-0.3				-230.9	-231.0	0.1
Diphenylethanedione (Benzil)	C14H10O2 (1)	134-81-6	-55.5	-52.7	-2.8				-153.9	-154.0	0.1
9,10-Epidioxyanthracene	C14H10O2 (2)	220-42-8							82.9	98.3	-15.4
2-Phenyl-1,4-benzodioxin	C14H10O2	5770-58-1	-62.8 S	-61.9	-0.8						
4b,10a-Dihydro-benzo[b]benzo[3,4]-cyclobuta[1,2-e][1,4]dioxin	C14H10O2	42896-18-4	-16.7 S	-16.3	-0.4						
2-Hydroxy-1,2-diphenylethanone (Benzoin)	C14H12O2 (1)	119-53-9							-247.7	-247.7	-0.0
3,5-Di-tert-butyl-1,2-benzenediol	C14H22O2 (1)		-470.5 P94	-478.6	8.1				-570.6 P94	-600.0	29.4
Tetradecanoic acid (Myristic acid)	C14H28O2 (1)	544-63-8	-693.7	-682.8	-10.9	-788.8	-787.4	-1.4	-833.5	-830.9	-2.6
Tridecanoic acid methyl ester	C14H28O2 (2)	1731-88-0	-635.4	-642.2	6.8	-717.9	-719.6	1.7			

Table 5. Carbon-Hydrogen-Oxygen compounds (CxHyO2): Enthalpy of formation (298 K), 10

Compound	Formula (PNK #)	CAS Registry No.	Gas			Liquid			Solid		
			Expt. Ref.	Calc.	Δ	Expt. Ref.	Calc.	Δ	Expt. Ref.	Calc.	Δ
Decanoic acid tert-butyl ester	C14H28O2 (3)	16474-41-2				-752.8	-763.6	10.8			
2,11-Dimethyl-2,11-dodecanediol	C14H30O2 (1)	22092-59-7							-846.2	-861.9	15.7
1,3-Diphenyl-1,3-propanedione	C15H12O2 (1)	120-46-7							-224.2	-263.6	39.4
2,2-Bis(4-hydroxyphenyl)-propane	C15H16O2 (1)	80-05-7							-368.6	-368.2	-0.4
3,5-Di-tert-butylbenzoic acid	C15H22O2 (1)	16225-26-6	-516.2	-509.6	-6.6				-624.6	-615.9	-8.7
Pentadecanoic acid	C15H30O2 (1)	1002-84-2	-699.0	-703.7	4.7	-811.7	-813.0	1.3	-861.7	-860.2	-1.5
Tetradecanoic acid methyl ester	C15H30O2 (2)	124-10-7	-656.5	-663.2	6.7	-743.9	-745.2	1.3			
1,4-Diphenyl-2-buten-1,4-dione	C16H12O2 (1)	4070-75-1							-114.7	-116.3	1.6
1,4-Diphenyl-1,4-butanedione	C16H14O2 (1)	495-71-6							-255.6	-352.3	96.7
Hexadecanoic acid (Palmitic acid)	C16H32O2 (1)	57-10-3	-737.1	-724.7	-12.4	-838.1	-838.5	0.4	-891.5	-889.5	-2.0
Pentadecanoic acid methyl ester	C16H32O2 (2)	7132-64-1	-680.0	-684.1	4.1	-771.0	-770.7	-0.3			
Dodecanoic acid tert-butyl ester	C16H32O2 (3)	7143-18-2				-817.8	-814.6	-3.2			
Benzoic acid 2-naphthyl ester	C17H12O2 (1)	93-44-7							-184.8	-192.0	7.2
1,3-Diphenyl-3-ethoxy-2-propen-1-one	C17H16O2 (1)	1907-69-3							-190.4	-190.4	-0.0
Heptadecanoic acid (Margaric acid)	C17H34O2 (1)	506-12-7				-865.6	-864.0	-1.6	-924.4	-918.8	-5.6
5,12-Naphthacenedione	C18H10O2 (1)	1090-13-7	-34.0	-27.6	-6.4				-142.8	-159.8	17.0
1,2-Benzanthracene-9,10-dione	C18H10O2 (2)		-149.0	-148.5	-0.5				-231.8	-231.8	-0.0
(Z,Z)-9,12-Octadecadienoic acid (Linoleic acid)	C18H32O2	2197-37-7				-674.0 SWS	-649.8	-24.3			
(Z)-9-Octadecenoic acid (Oleic acid)	C18H34O2	2027-47-6							-802.5 SWS	-817.6	15.1
Octadecanoic acid (Stearic acid)	C18H36O2 (1)	57-11-4	-781.2	-766.5	-14.7	-884.7	-889.5	4.8	-947.7	-948.1	0.4
Tetradecanoic acid tert-butyl ester	C18H36O2 (2)	32429-42-8				-862.7	-865.7	3.0			
(Z)-9-Octadecenoic acid methyl ester	C19H36O2 (1)	112-62-9	-649.9	-625.9	-24.0	-734.5	-731.8	-2.7			
(E)-9-Octadecenoic acid methyl ester	C19H36O2 (2)	1937-62-8				-737.0	-735.5	-1.5			
Nonadecanoic acid	C19H38O2 (1)	646-30-0	-785.3	-787.4	2.1	-916.4	-915.0	-1.4	-984.0	-977.4	-6.6
2,3-Diphenylbenzo-1,4-dioxin	C20H14O2	75694-46-1	37.7 S	38.9	-1.3						
(Z)-9-Octadecenoic acid ethyl ester	C20H38O2 (1)	111-62-6				-775.8	-769.9	-5.9			
(E)-9-Octadecenoic acid ethyl ester	C20H38O2 (2)	6114-18-7				-773.2	-773.6	0.4			
Eicosanoic acid (Arachidic acid)	C20H40O2 (1)	506-30-9	-812.4	-808.3	-4.1	-940.0	-940.6	0.6	-1011.9	-1006.7	-5.2
(Z)-9-Octadecenoic acid propyl ester	C21H40O2 (1)	111-59-1				-792.3	-795.4	3.1			
(E)-9-Octadecenoic acid propyl ester	C21H40O2 (2)	58930-02-2				-798.6	-799.1	0.5			
6,13-Pentacenedione	C22H12O2 (1)	3029-32-1	43.5	44.4	-0.9				-72.8	-107.1	34.3
(E)-13-Docosenoic acid	C22H42O2 (1)	506-33-2							-960.7	-968.2	7.5
(Z)-9-Octadecenoic acid butyl ester	C22H42O2 (2)	142-77-8				-816.9	-817.1	0.2			
(E)-9-Octadecenoic acid butyl ester	C22H42O2 (3)	22147-33-7				-823.6	-820.9	-2.7			
(E)-9-Octadecenoic acid pentyl ester	C23H44O2 (1)	58930-03-3				-850.6	-846.4	-4.2			
Benzo[rst]pentaphene-5,8-dione	C24H12O2 (1)	3302-52-1	-138.5	-138.1	-0.4				-251.1	-250.6	-0.5
Bis(triphenylmethyl)peroxide	C38H30O2 (1)	596-30-5							321.4	319.7	1.7
5,12,6,11-Bisepidioxy-5,6,11,12-tetrahydro-5,6,11,12-tetraphenyl-naphthacene	C42H28O2 (1)								278.4	279.1	-0.7
5,12-Dihydro-5,6,11,12-tetraphenyl-	C42H28O2 (2)	32287-37-9							516.6	516.3	0.3

Table 5. Carbon-Hydrogen-Oxygen compounds (CxHyO2): Enthalpy of formation (298 K), 11

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
5,12-epidioxy-naphthacene 4b,9-Dihydro-9-hydroperoxy-4b,9,10-triphenyl-indeno-[1,2,3-fg]naphthacene-9-yl	C42H28O2 (3)	38118-83-1									607.7		609.0	-1.3

Notes and References

a: 47BIE/TRU: Bieber and Trumpler, Helv. Chim Acta, 30, 1860 (1947). As cited in 52BEL/CLU.
b: 52BEL/CLU: R. P. Bell and J. C. Clunie, Trans. Faraday Soc. 48, 439 (1952). Calculated from heat of hydration of CH3CHO in dilute aqueous solution at 298 K.
c: Gas phase value calculated from liquid value and ΔHvap recommended by V. Majer and V. Svoboda, "Enthalpies of Vaporization of Organic Compounds," Blackwell Scientific Publs., 1985.
d: J. Font and J. Mutasell, Thermochim. Acta 246, 57 (1994) measured ΔHsubl. at 311 K from the crystalline phase.
e: 67PIH/HEI: K. Pihlaja and J. Heikkila, Acta Chem. Scand. 21, 3290 (1967).
f: 88RIB/RIB: M. D. M. C. Ribeiro Da Silva, M. A. V. Ribeiro Da Silva, and G. Pilcher, J. Chem. Thermodyn. 20, 969 (1988).
g: 81FER/DAS: M. L. C. C. H. Ferrao, M. A. V. Ribeiro da Silva, S. Suradi, G. Pilcher, and H. A. Skinner, J. Chem. Thermodyn. 13, 567 (1981).
h: 88COLI/JIM: M. Colomina, P. Jimenez, R. Perez-Ossorio, M. V. Roux, and C. Turrion, J. Chem. Thermodyn. 20, 575 (1988).
i: 69PIH/LAU: K. Pihlaja and T. Laurosalo, Acta Chem. Scand. 23, 3264 (1969); gas phase values calculated from estimated heats of vaporization.
*: PNK values based on 72GAR/HUS. They also cite 37MOU/DOD, who report -123.1 for liquid, which would give -106.8 for gas.
**: CP give -104.6 (g) and -119.6 kcal/mol (l), citing 37MOU/DOD.

CP: J. D. Cox and G. Pilcher, "Thermochemistry of Organic and Organometallic Compounds," Academic Press, 1970.
DH: E. S. Domalski and E. D. Hearing, "Estimation of Thermodynamic Properties of C-H-N-O-S-Halogen Compounds at 298.15 K," J. Phys. Chem. Ref. Data 22, 805 (1993).
G: J. P. Guthrie, "Thermodynamics of enols," Ch. 2 in "The Chemistry of Enols," Z Rappoport, ed. (Wiley, 1990).
L: S. G. Lias, J. E. Bartmess, J. F. Liebman, J. L. Holmes, R. D. Levin, and W. G. Mallard, "Gas-Phase Ion and Neutral Thermochemistry," J. Phys. Chem. Ref. Data 17 (Supplement 1), 1988.
P: G. Pilcher, "Thermochemistry of carboxylic acids and derivatives," Ch. 2 in Supplement B: The Chemistry of Acid Derivatives, Vol. 2 (Wiley, 1992)
P94: J. B. Pedley, "Thermochemical Data and Structures of Organic Compounds, Vol. 1" (TRC Data Series, 1994).
S: S. E. Stein, J. M. Rukkers, and R. L. Brown, "NIST Structures & Properties Database and Estimation Program, NIST-SRD DB 25," Version 2.0 (1994).
SWS: D. R. Stull, E. F. Westrum, Jr., and G. C. Sinke, "The Chemical Thermodynamics of Organic Compounds" (Krieger, 1987).

Table 6. Carbon-Hydrogen-Oxygen compounds (CxHyO3): Enthalpy of formation (298 K), 1

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
1,3-Dioxol-2-one	C3H2O3 (1)	872-36-6	-418.6		-413.4	-5.2	-459.9		-472.8	12.9				
1,3-Dioxolan-2-one (Ethylene carbonate)	C3H4O3 (1)	96-49-1	-508.4		-508.4	-0.0	-571.5		-575.7	4.2	-581.6		-581.6	-0.0
2-Oxo-propanoic acid	C3H4O3	127-17-3	-548.1	S	-533.5	-14.6								
1,3,5-Trioxane (Trioxymethylene)	C3H6O3 (1)	110-88-3	-465.9		-492.9	27.0					-522.5		-522.6	0.1
(S)-2-Hydroxypropanoic acid (Lactic acid)	C3H6O3 (2)	79-33-4									-694.0		-685.8	-8.2
1,2,3-Propanetriol (Glycerol)	C3H8O3 (1)	56-81-5	-577.8	P94	-573.6	-4.2	-669.4	P94	-675.6	7.1				
2,5-Furandione (Maleic anhydride)	C4H2O3 (1)	108-31-6	-398.3		-405.4	7.1					-469.8		-482.4	12.6
Dihydro-2,5-furandione (Succinic anhydride)	C4H4O3 (1)	108-30-5	-527.9	DH	-528.0	0.1	-588.6	DH	-579.9	-8.7	-608.6	DH	-601.7	-6.9
Acetic anhydride	C4H6O3 (1)	108-24-7	-572.5		-571.5	-1.0	-624.4		-637.6	13.2				
4-Methyl-1,3-cioxolan-2-one (Propylene carbonate)	C4H6O3 (2)	108-32-7	-582.5		-546.4	-36.1	-613.2		-615.5	2.3				
2,2'-Oxybisethanol (Diethylene glycol)	C4H10O3 (1)	111-46-6	-571.2		-552.3	-18.9	-628.5		-638.1	9.6				
Trimethoxymethane	C4H10O3 (2)	149-73-5	-531.9		-536.4	4.5	-570.0		-566.5	-3.5				
2-Furancarboxylic acid (Furoic acid)	C5H4O3 (1)	25447-28-9	-389.9		-397.5	7.6					-498.4		-506.2	7.8
3-Methyl-2,5-furandione	C5H4O3 (2)	616-02-4	-447.2		-437.6	-9.6	-504.5		-504.6	0.1				
3-Furancarboxylic acid	C5H4O3	488-93-7	-389.1	S	-403.8	14.6								
3,4-Dihydro-3-methyl-2,5-furandione	C5H6O3 (1)	4100-80-5					-617.6		-612.5	-5.1	-620.0		-620.5	0.5
Glutaric anhycride	C5H6O3	108-55-4	-532.4	DH	-532.2	-0.2					-618.5	DH	-618.4	-0.1
Carbonic acid diethyl ester	C5H10O3 (1)	105-58-8	-637.9		-637.2	-0.7	-681.5		-671.1	-10.4				
1,3,6-Trioxacyclooctane	C5H10O3 (2)	177-91-9	-467.1		-466.9	-0.2	-515.9		-515.9	-0.0				
2-(Hydroxymethyl)-2-methyl-1,3-propanediol	C5H12O3 (1)	7-78-5									-744.6		-738.9	-5.7
1,1,1-Trimethoxyethane (Trimethyl orthoacetate)	C5H12O3 (2)	1445-45-0	-572.7		-572.8	0.1	-612.0		-612.5	0.5				
3,4-Dimethyl-2,5-furandione	C6H6O3 (1)	766-39-2									-581.4		-551.9	-29.5
2-Furancarboxylic acid methyl ester	C6H6O3 (2)	611-13-2	-404.8		-377.8	-27.0	-450.0		-436.0	-14.0				
1,2,3-Benzenetriol	C6H6O3 (3)	87-66-1	-434.3	P94	-448.9	14.6					-551.0	P94	-567.4	16.3
1,2,4-Benzenetriol	C6H6O3 (4)	533-73-3	-443.9	P94	-451.0	7.1					-564.0	P94	-573.6	9.6
1,3,5-Benzenetriol	C6H6O3 (5)	108-73-6	-453.1	P94	-453.1	-0.0					-584.5	P94	-579.9	-4.6
Dihydro-3,3-dimethyl-2,5-furandione	C6H8O3 (1)	17347-61-4	-581.7		-584.1	2.4	-645.5		-640.6	-4.9	-651.4		-646.8	-4.6
(Z)-3,4-Dihydro-3,4-dimethyl-2,5-furandione	C6H8O3 (2)	13844-07-8									-658.0		-637.6	-20.4
(E)-3,4-Dihydro-3,4-dimethyl-2,5-furandione	C6H8O3 (3)	35392-94-0									-667.2		-639.3	-27.9
Dihydro-3-ethyl-2,5-furandione	C6H8O3 (4)	14035-81-5					-642.4		-638.1	-4.3				
Propanoic anhydride	C6H10O3 (1)	123-62-6	-626.5		-615.0	-11.5	-679.1		-681.2	2.1				
2,4,6-Trimethyl-1,3,5-trioxane (Paraldehyde)	C6H12O3 (1)	123-63-7	-631.8		-609.6	-22.2	-673.2		-671.1	-2.1				
2,3-Butanediol monoacetate	C6H12O3 (2)	56255-48-2					-719.6		-740.1	20.5				
Propanoic acid ethoxymethyl ester	C6H12O3 (4)	54078-53-4	-617.3		-635.5	18.2	-667.2		-677.0	9.8				
2-Ethyl-2-(hydroxymethyl)-1,3-propanediol	C6H14O3 (1)	77-99-6									-750.9		-764.8	13.9
3,5,7-Trioxanonane	C6H14O3 (2)	93-59-4	-581.1		-588.3	7.2	-625.8		-627.2	1.4				
Benzenecarbcperoxoic acid (Perbenzoic acid)	C7H6O3 (1)	69-72-7									-367.0		-285.1	-81.9
2-Hydroxybenzoic acid (Salicylic acid)	C7H6O3 (2)	539-47-9	-494.8		-467.4	-27.4					-589.9		-579.1	-10.8
3-Hydroxybenzoic acid	C7H6O3										-584.9	SWS	-583.2	-1.7
4-Hydroxybenzoic acid	C7H6O3										-584.5	SWS	-583.2	-1.3
3-(2-Furanyl)-2-propenoic acid	C7H6O3 (3)	281-32-3									-459.0		-455.2	-3.8

Table 6. Carbon-Hydrogen-Oxygen compounds (CxHyO3): Enthalpy of formation (298 K), 2

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
1,3-Dihydroxy-3-methoxybenzene	C7H8O3 (1)		-418.5	P94	-418.0	-0.5					-510.2	P94	-542.7	32.5
Dihydro-3,3,4-trimethyl-2,5-furandione	C7H10O3 (2)	35046-67-4	-614.3		-611.3	-3.0					-688.4		-665.7	-22.7
Triethoxymethane	C7H16O3 (1)	122-510	-635.3		-638.1	2.8	-681.3		-680.7	-0.6				
1,3-Isobenzofurandione (Phthalic anhydride)	C8H4O3 (1)	85-44-9	-371.4		-371.1	-0.3					-460.1		-460.2	0.1
3-Hydroxy-4-methoxy-benzaldehyde	C8H8O3 (1)	621-59-0									-453.4		-461.5	8.1
2,4-Dihydroxyacetophenone	C8H8O3 (2)	89-84-9									-573.5		-564.8	-8.7
(R,S)-a-Hydroxybenzene-acetic acid	C8H8O3 (3)	611-72-3									-579.4		-580.3	0.9
(S)-a-Hydroxybenzene-acetic acid	C8H8O3 (4)	17199-29-0									-580.6		-580.3	-0.3
2-Methoxybenzoic acid	C8H8O3 (5)	579-75-9	-433.8		-438.5	4.7					-538.5		-560.7	22.2
3-Methoxybenzoic acid	C8H8O3 (6)	586-38-9	-446.1		-451.0	4.9					-553.5		-564.8	11.3
4-Methoxybenzoic acid	C8H8O3 (7)	100-09-4	-451.9		-451.0	-0.9					-561.7		-564.8	3.1
Salicylic acid methyl ester	C8H8O3						-531.8	SWS	-539.6	7.8				
Dihydro-3,3,4,4-tetramethyl-2,5-furandione	C8H12O3 (1)	35046-68-5									-691.9		-692.0	0.1
Dihydro-3,3-diethyl-2,5-furandione	C8H12O3 (2)	2840-69-9									-688.8		-705.4	16.6
(Z)-Dihydro-3,4-diethyl-2,5-furandione	C8H12O3 (3)	35046-84-5									-693.4		-696.2	2.8
(E)-Dihydro-3,4-diethyl-2,5-furandione	C8H12O3 (4)	35046-86-7					-700.0		-696.2	-3.8				
2-Ethyl-3-oxobutanoic acid ethyl ester	C8H14O3 (1)	607-97-6	-659.7		-630.5	-29.2	-716.6		-699.3	-17.3				
3-Ethoxy-2-butenoic acid ethyl ester	C8H14O3 (2)	998-91-4					-647.0		-607.1	-39.9				
Carbonic acid cyclohexylmethyl ester	C8H14O3 (3)	25066-36-8	-663.2		-692.9	29.7	-708.8		-766.5	57.7				
2-(2-Methoxyethoxy)-tetrahydro-2H-pyran	C8H16O3 (1)	4819-82-3	-563.0		-566.5	3.5	-623.3		-622.6	-0.7				
(3aa,4a,7a,7aa)-3a,4,7,7a-Tetrahydro-4,7-methano-... isobenzofuran-1,3-dione	C9H8O3 (1)	129-64-6	-374.8		-374.5	-0.3					-471.8		-471.5	-0.3
3-(2-Hydroxyphenyl)-2-propenoic acid	C9H8O3	614-60-8	-431.0	S	-409.6	-21.3								
1-tert-Butoxy-3-ethoxy-2-propanol	C9H20O3 (1)	42910-64-5					-750.7		-761.5	10.8				
Dihydro-3-phenyl-2,5-furandione	C10H8O3 (1)	1131-15-3									-501.5		-492.9	-8.6
(E)-3-(2-Methoxyphenyl)-2-propenoic acid	C10H10O3	1011-54-7	-393.3	S	-380.7	-12.6								
Dihydro-3,3,4-triethyl-2,5-furandione	C10H16O3 (1)										-745.6		-753.5	7.9
2,2-Dimethylpropanoic anhydride	C10H18O3 (1)	1538-75-6					-780.0		-802.5	22.5				
1-tert-Butoxy-3-propoxy-2-propanol	C10H22O3 (1)	42991-60-6					-774.0		-787.0	13.0				
3-Hydroxy-2-naphthoic acid	C11H8O3 (1)	92-70-6									-547.8		-531.4	-16.4
1-Butoxy-3-tert-butoxy-2-propanol	C11H24O3 (1)	42910-65-6					-794.3		-812.5	18.2				
Dihydro-3,3,4,4-tetraethyl-2,5-furandione	C12H20O3 (1)	35046-71-0									-799.4		-809.2	9.8
Dodecaneperoxoic acid	C12H24O3 (1)	2388-12-7									-680.3		-680.1	-0.2
1-(tert-Butoxy)-3-pentoxy-2-propanol	C12H26O3 (1)	42910-66-7					-818.0		-838.1	20.1				
Phenyl 2-hydroxybenzoate (Phenyl salicylate)	C13H10O3 (1)	118-55-8	-344.5		-326.4	-18.1					-436.6		-445.6	9.0
Carbonic acid diphenyl ester	C13H10O3 (2)	102-09-0	-311.2		-301.7	-9.5	-377.7		-364.8	-12.9	-401.2		-376.6	-24.6
1,5-Bis(2-furyl)-1,4-pentadien-3-one	C13H10O3 (3)	886-77-1									-201.1		-233.4	32.3
Carbonic acid dicyclohexyl ester	C13H22O3 (1)	4427-97-8	-763.7		-749.4	-14.3					-830.2		-807.5	-22.7
Benzoic anhydride	C14H10O3 (1)	93-97-0	-319.0		-312.1	-6.9	-377.7		-413.4	35.7	-415.4		-454.4	39.0
3,5-Diphenyl-1,2,4-trioxolane	C14H12O3 (1)	23888-15-5									-123.8		-107.1	-16.7
Tetradecaneperoxoic acid (Pertetradecanoic acid)	C14H28O3 (1)	19816-73-0									-749.9		-677.6	-72.3

Table 6. Carbon-Hydrogen-Oxygen compounds (CxHyO3): Enthalpy of formation (298 K), 3

Compound	Formula (PNK #)	CAS Registry No.	Gas			Liquid			Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
Decaneperoxoic acid tert-butyl ester	C14H28O3 (2)	16474-36-5					-688.4		-690.4	2.0				
Santonin	C15H18O3 (1)	481-06-1									-590.8		-567.4	-23.4
b-Santonin	C15H18O3 (2)	481-07-2									-587.3		-567.4	-19.9
6-a(H)-Santonin	C15H18O3 (3)										-584.9			
6,11-a(H)-Santonin	C15H18O3 (4)										-603.0			
(E)-Dihydro-3,4-diphenyl-2,5-furandione	C16H12O3 (1)	5465-38-3									-419.9		-428.4	8.5
2-Methylbenzoic acid anhydride (o-Toluic anh.)	C16H14O3 (1)	607-86-3									-533.5		-518.8	-14.7
4-Methylbenzoic acid anhydride	C16H14O3 (2)	13222-85-0									-521.0		-527.2	6.2
Benzenecarboperoxoic acid 1-methyl-1-phenylethyl ester (Cumyl perbenzoate)	C16H16O3 (1)		-188.4		-165.7	-22.7					-231.5		-197.1	-34.4
Hexadecaneperoxoic acid (Perhexadecanoic acid)	C16H32O3 (1)	7311-29-7									-801.9		-736.2	-65.7
Dodecaneperoxoic acid tert-butyl ester	C16H32O3 (2)	2123-88-8					-738.3		-741.4	3.1				
3-Phenyl-2-propenoic anhydride (Cinnamic anh.)	C18H14O3 (1)	538-56-7									-347.8		-353.1	5.3
Octadecaneperoxoic acid (Perstearic acid)	C18H36O3 (1)	5796-86-1									-857.3		-794.8	-62.5
Tetradecaneperoxoic acid tert-butyl ester	C18H36O3 (2)	59710-71-3					-795.8		-792.4	-3.4				
Carbonic acid bis-((4-biphenyl)methyl) ester	C27H22O3 (1)		-209.2		-207.9	-1.3					-320.9		-320.5	-0.4
Oxalic acid (Ethanedioic acid)	C2H2O4 (1)	144-62-7	-723.7		-730.5	6.8					-821.7		-815.0	-6.7
Bis(hydroxymethyl)-peroxide (Dioxybismethanol)	C2H6O4 (1)	17088-73-2	-571.7		-497.1	-74.6					-665.8		-665.3	-0.5
Propanedioic acid (Malonic acid)	C3H4O4 (1)	141-82-2									-891.0		-844.3	-46.7
2-Butynedioic acid	C4H2O4 (1)	142-45-0									-577.4		-584.9	7.5
3,4-Dihydroxy-3-cyclobutene-1,2-dione	C4H2O4 (2)	2892-51-5									-598.2		-598.3	0.1
Maleic acid ((Z)-2-Butenedioic acid)	C4H4O4 (1)	110-16-7	-679.4		-709.6	30.2					-789.4		-789.9	0.5
Fumaric acid ((E)-2-Butenedioic acid)	C4H4O4 (2)	110-17-8	-675.8		-705.0	29.2					-812.2	DH	-785.8	-26.4
Diacetyl peroxide	C4H6O4 (1)	110-22-5					-535.3		-589.9	54.6				
Butanedioic acid (Succinic acid)	C4H6O4 (2)	110-15-6	-823.0		-821.7	-1.3					-940.5		-933.0	-7.5
Ethanedioic acid dimethyl ester	C4H6O4 (3)	553-90-2	-708.9		-691.2	-17.7	-735.2	DH	-734.7	-0.5	-756.3		-754.0	-2.3
1,3,5,7-Tetroxane	C4H8O4 (1)	293-30-1	-620.2		-620.1	-0.1					-699.9		-700.0	0.1
2(R),3(S)-1,2,3,4-Butanetetrol (l-Erythritol)	C4H10O4 (1)	149-32-6	-775.2		-762.3	-12.9	-887.0		-896.2	9.2	-910.4		-887.0	-23.4
(E)-2-Methyl-2-butenedioic acid (Mesaconic acid)	C5H6O4 (1)	498-24-8									-824.4		-824.7	0.3
Methylenebutanedioic acid (Itaconic acid)	C5H6O4 (2)	97-65-4									-841.1		-830.5	-10.6
(Z)-2-Methyl-2-butenedioic acid (Citraconic acid)	C5H6O4	498-23-7									-824.7	SWS	-824.7	
Methylbutanedioic acid (Methylsuccinic acid)	C5H8O4 (1)	498-21-5									-958.2		-950.2	-8.0
Pentanedioic acid (Glutaric acid)	C5H8O4 (2)	110-94-1									-960.0		-962.3	2.3
Ethylmalonic acid	C5H8O4										-941.0	SWS	-941.0	
1,2,3-Propanetriol monoacetate (Glycerol 1-acetate)	C5H10O4 (1)	26446-35-5					-909.2		-880.3	-28.9				
2-Deoxy-D-ribose	C5H10O4 (2)	533-67-5									-869.4	P94		
3-(2-Hydroxyethoxy)-1,2-propanediol	C5H12O4 (1)	14641-24-8					-863.4		-857.7	-5.7				
2,2-Bis(hydroxymethyl)-1,3-propanediol (Pentaerythritol)	C5H12O4 (2)	115-77-5	-776.7		-770.3	-6.4					-920.6		-926.8	6.2

Table 6. Carbon-Hydrogen-Oxygen compounds (CxHyO3): Enthalpy of formation (298 K), 4

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
Tetramethoxymethane (Tetramethyl orthocarbonate	C5H12O4	1850-14-2	-727.2	DH	-727.2	-0.0	-767.1	DH	-767.8	0.7				
2,2-Dimethylbutanedioic acid	C6H10O4(1)	597-43-3									-987.8		-974.9	-12.9
meso-2,3-Dimethylbutanedioic acid	C6H10O4(2)	608-39-9									-977.5		-965.7	-11.8
racemic-2,3-Dimethylbutanedioic acid	C6H10O4(3)	608-40-1									-983.8		-965.7	-18.1
(-)-2,3-Dimethylbutanedioic acid	C6H10O4(4)	57694-62-9									-982.5		-965.7	-16.8
2-Ethylbutanedioic acid	C6H10O4(5)	636-48-6									-989.2		-979.5	-9.7
Hexanedioic acid (Adipic acid)	C6H10O4(6)	124-04-9	-865.0		-863.6	-1.4					-994.3		-991.6	-2.7
Ethanedioic acid diethyl ester	C6H10O4(7)	95-92-1	-742.0		-759.0	17.0	-805.5		-810.9	5.4				
Bis(1-oxypropyl) peroxide (Dipropionyl peroxide)	C6H10O4(8)	3248-28-0					-620.0		-633.5	13.5				
5-(1a,2b,3b,4a,)-1,2,3,4-Cyclohexenetetrol	C6H10O4(9)	526-87-4									-836.3		-836.0	-0.3
Propylmalonic acid	C6H10O4										-965.2	SWS	-970.3	5.0
1,2-Bis(2-hydroxyethoxy)-ethane (Triethylene glycol)	C6H14O4(1)	112-27-6	-725.0		-719.6	-5.4	-804.2		-819.2	15.0				
Trimethylbutanedioic acid	C7H12O4(1)	2103-16-4									-1000.8		-988.7	-12.1
Heptanedioic acid (Pimelic acid)	C7H12O4(2)	111-16-0									-1009.4		-1020.9	11.5
2,4,8,10-Tetraoxospiro-[5.5]undecane	C7H12O4(3)	126-54-5	-629.5		-629.7	0.2					-702.3		-702.5	0.2
Butylmalonic acid	C7H12O4										-996.2	SWS	-999.6	3.3
3,5,7,9-Tetraoxaundecane	C7H16O4(1)	4431-82-7	-741.0		-756.9	15.9	-794.6		-801.7	7.1				
3-(tert-Butyldioxy)-1,2-propanediol	C7H16O4(3)	38578-50-6					-719.1		-707.1	-12.0				
1,2-Benzenedicarboxylic acid (Phthalic acid)	C8H6O4 (1)	88-99-3									-782.0		-766.9	-15.1
1,3-Benzenedicarboxylic acid (Isophthalic acid)	C8H6O4 (2)	121-91-5	-696.3		-685.3	-11.0					-803.0		-792.4	-10.6
1,4-Benzenedicarboxylic acid (Terephthalic acid)	C8H6O4 (3)	100-21-0	-717.9		-685.3	-32.6					-816.1		-792.4	-23.7
3,4-Diethoxy-3-cyclobutene-1,2-dione	C8H10O4(1)	5231-87-8	-478.5		-478.6	0.1	-552.1		-553.1	1.0				
(Z)-Cyclohexane-1,2-dicarboxylic acid	C8H12O4(1)	610-09-3									-961.1		-998.3	37.2
(E)-Cyclohexane-1,2-dicarboxylic acid	C8H12O4(2)	2305-32-0									-970.7		-1003.3	32.6
Tetramethylbutanedioic acid	C8H14O4(1)	630-51-3									-1012.4		-1010.0	-2.4
2,2-Diethylbutanedioic acid	C8H14O4(2)	5692-97-7									-1032.7		-1026.8	-5.9
meso-2,3-Diethylbutane-dioic acid	C8H14O4(3)	35392-80-4									-1019.2		-1025.9	6.7
racemic-2,3-Diethylbutane-dioic acid	C8H14O4(4)	35392-77-9									-1026.3		-1025.9	-0.4
Octanedioic acid (Suberic acid)	C8H14O4(5)	505-48-6	-894.9		-905.4	10.5					-1038.0		-1050.2	12.2
2,3-Butanedioldiacetate	C8H14O4(6)	1114-92-7					-916.3		-943.9	27.6				
Bis(1-oxobutyl)peroxide	C8H14O4(7)	2697-95-2					-673.2		-684.5	11.3				
Pentylmalonic acid	C8H14O4										-1020.9	SWS	-1028.8	7.9
Dimethyl dimethoxysuccinate, dl	C8H14O4										-1110.0	SWS	-1101.2	-8.8
Dimethyl dimethoxysuccinate, meso	C8H14O4										-1153.5	SWS	-1101.2	-52.3
1,4,7,10-Tetraoxacyclododecane (12-Crown-4)	C8H16O4(1)	294-93-9	-631.0		-630.9	-0.1	-696.6		-696.6	0.0				
1-(tert-Butyldioxy)-3-methoxy-2-propanol	C8H18O4(2)	38578-20-0					-666.3		-670.3	4.0				
4-Methyl-2H,7H-pyrano-[2,3-b]pyran-2,7-dione	C9H6O4 (1)	37831-57-5									-387.1		-457.3	70.2
7-Methyl-2H,5H-pyrano-[4,3-b]pyran-2,5-dione	C9H6O4 (2)	7316-90-7									-450.1		-457.3	7.2
2-Acetoxybenzoic acid (Acetylsalicylic acid)	C9H8O4 (1)	50-78-2									-815.6	a	-720.9	-94.7

Table 6. Carbon-Hydrogen-Oxygen compounds (CxHyO3): Enthalpy of formation (298 K), 5

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
2,3-Dimethoxybenzoic acid	C9H10O4 (1)		-570.4	P94	-575.7	5.3					-687.0	P94	-738.5	51.5
2,6-Dimethoxybenzoic acid	C9H10O4 (3)		-572.1	P94	-575.7	3.6					-693.8	P94	-743.9	50.1
3,4-Dimethoxybenzoic acid	C9H10O4 (4)		-584.2	P94	-588.3	4.1					-714.0	P94	-742.7	28.7
2,4-Dimethoxybenzoic acid	C9H10O4 (2)		-588.8	P94	-588.3	-0.5					-712.2	P94	-748.1	35.9
3,5-Dimethoxybenzoic acid	C9H10O4 (5)		-596.9	P94	-600.8	3.9					-724.0	P94	-752.3	28.3
(Z)-1,2-Cyclopentylene diacetate	C9H14O4						-879.5	SWS	-899.1	19.7				
(E)-1,2-Cyclopentylene diacetate	C9H14O4						-882.8	SWS	-900.8	18.0				
Nonanedioic acid	C9H16O4 (1)	123-99-9									-1054.3		-1079.5	25.2
Butanedioic acid tert-butyl methyl ester	C9H16O4 (2)	14734-25-9					-950.9		-952.3	1.4				
Hexylmalonic acid	C9H16O4										-1049.8	SWS	-1058.1	8.4
1-(tert-Butyldioxy)-3-ethoxy-2-propanol	C9H20O4 (1)	36578-21-1					-706.7		-708.4	1.7				
Tetraethoxymethane	C9H20O4 (2)	78-09-1	-860.6	P94	-862.7	2.1	-913.6	P94	-920.1	6.5				
5,8-Dihydroxy-1,4-naphthalenedione	C10H6O4 (1)		-499.1	P94	-483.3	-15.8					-595.1	P94	-595.4	0.3
4,5-Dimethyl-2H,7H-pyrano-[2,3-b]-pyran-2,7-dione	C10H8O4 (1)	37831-60-0									-564.4		-487.0	-77.4
4,7-Dimethyl-2H,5H-pyrano-[4,3-b]-pyran-2,5-dione	C10H8O4 (2)	1204-38-2									-436.4		-459.4	23.0
4,6-Dimethylpyrano[3,2-b]-pyran-2,8-dione	C10H8O4 (3)	33759-64-7									-527.4		-528.4	1.0
Phenylbutanedioic acid (Phenylsuccinic acid)	C10H10O4 (1)	635-51-8									-841.0		-824.2	-16.8
2,4-Diacetyl-1,3-benzenediol	C10H10O4 (2)	2163-12-4									-753.5		-751.4	-2.1
4,6-Diacetyl-1,3-benzenediol	C10H10O4 (3)	2161-85-5									-776.5		-755.6	-20.9
1,3-Benzenedicarboxylic acid dimethyl ester	C10H10O4 (4)	1459-93-4									-730.9		-731.4	0.5
1,4-Benzenedicarboxylic acid dimethyl ester	C10H10O4 (5)	120-61-6									-732.6		-731.4	-1.2
1,2,3-Propanetriol 1-benzoate	C10H12O4 (1)	3376-59-8									-777.3		-769.0	-8.3
1,2,3-Propanetriol 2-benzoate	C10H12O4 (2)										-772.8		-769.0	-3.8
(Z)-Cyclohexane-1,3-dicarboxylic acid dimethyl ester	C10H16O4 (1)	6998-82-9					-846.5		-905.0	58.5				
(E)-Cyclohexane-1,3-dicarboxylic acid dimethyl ester	C10H16O4 (2)	10021-92-8					-854.5		-900.4	45.9				
Triethylbutanedioic acid	C10H18O4 (1)	2103-18-6									-1066.3		-1068.2	1.9
Decanedioic acid (Sebacic acid)	C10H18O4 (2)	111-20-6	-921.9		-947.3	25.4					-1082.6		-1108.8	26.2
Heptylmalonic acid	C10H18O4										-1078.2	SWS	-1087.4	9.2
1-(tert-Butyldioxy)-3-propoxy-2-propanol	C10H22O4 (1)	36578-22-2					-725.0		-733.9	8.9				
Undecanedioic acid	C11H20O4 (1)	1852-04-6									-1099.4		-1138.0	38.6
Octylmalonic acid	C11H20O4										-1108.3	SWS	-1116.7	8.4
1-Butoxy-1-tert-butyldioxy-2-propanol	C11H24O4 (1)	36578-23-3					-747.0		-759.4	12.4				
1,2-Benzenedicarboxylic acid diethyl ester (Diethyl phthalate)	C12H14O4 (1)	84-66-2	-688.4		-688.7	0.3	-776.6		-759.2	-17.4				
(Z)-Cyclohexane-1,3-dicarboxylic acid diethyl ester	C12H20O4 (1)	62059-56-7					-933.7		-943.1	9.4				
(E)-Cyclohexane-1,3-dicarboxylic acid diethyl ester	C12H20O4 (2)	62059-57-8					-941.2		-943.1	1.9				
Tetraethylbutanedioic acid	C12H22O4 (1)	4111-60-8									-1096.5		-1113.8	17.3
Dodecanedioic acid	C12H22O4 (2)	693-23-2	-976.9		-989.1	12.2					-1130.0		-1167.3	37.3
Nonylmalonic acid	C12H22O4										-1138.0	SWS	-1146.0	7.9

Table 6. Carbon-Hydrogen-Oxygen compounds (CxHyO3): Enthalpy of formation (298 K), 6

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
1-(tert-Butyldioxy)-3-pentyloxy-2-propanol	C12H26O4 (1)	3578-71-1					-771.2		-784.9	13.7				
(E)-1,2-Indanylene diacetate	C13H14O4										-759.8	SWS	-707.1	-52.7
(Z)-1,2-Indanylene diacetate	C13H14O4										-774.5	SWS	-704.6	-69.9
Tridecanedioic acid	C13H24O4 (1)	505-52-2									-1148.3		-1196.6	48.3
Decylmalonic acid	C13H24O4										-1167.8	SWS	-1175.3	7.5
1,2,3-Propanetriol 1-decanoate	C13H26O4 (1)										-1109.0		-1105.4	-3.6
1,2,3-Propanetriol 2-decanoate	C13H26O4 (2)										-1095.7		-1105.4	9.7
1,4,9,10-Anthradiquinone	C14H6O4 (1)		-209.0	P94	-209.2	0.2					-333.0	P94	-333.0	0.0
Dibenzoyl peroxide	C14H10O4 (1)	94-36-0	-271.7		-271.1	-0.6					-369.6		-369.9	0.3
Oxalic acid diphenyl ester	C14H10O4 (2)	3155-16-6	-437.2		-423.4	-13.8	-508.3		-504.6	-3.7	-539.7		-539.7	0.0
1,4-Dihydroxy-9,10-anthraquinone	C14H8O4 (1)		-471.7	P94	-451.9	-19.8					-595.8	P94	-619.2	
1,2-Benzenedicarboxylic acid di-2-propenyl ester	C14H14O4 (1)	131-17-9					-551.5		-547.5	-4.0				
(Z)-1,2,3,4-Tetrahydro-1,2-naphthylene diacetate	C14H16O4										-812.5	SWS	-769.0	-43.5
(E)-1,2,3,4-Tetrahydro-1,2-naphthylene diacetate	C14H16O4										-819.2	SWS	-769.0	-50.2
Undecylmalonic acid	C14H26O4										-1197.5	SWS	-1204.6	7.1
Dodecylmalonic acid	C15H28O4										-1229.3	SWS	-1233.9	4.6
1,2,3-Propanetriol 1-dodecanoate	C15H30O4 (1)	142-18-7									-1160.9		-1164.0	3.1
1,2,3-Propanetriol 2-dodecanoate	C15H30O4 (2)	1678-45-1									-1152.6		-1164.0	11.4
meso-2,3-Diphenylbutanedioic acid	C16H14O4 (1)	1225-13-4									-733.5		-727.6	-5.9
racemic-2,3-Diphenylbutanedioic acid	C16H14O4 (2)	7584-72-7									-740.1		-727.6	-12.5
Bis(2-methylbenzoyl)-peroxide	C16H14O4 (3)	3034-79-5									-500.5		-437.6	-62.9
Bis(4-methylbenzoyl)-peroxide	C16H14O4 (4)	895-85-2									-451.5		-442.7	-8.8
(Z)-1-Phenyl-1,2-cyclohexylene diacetate	C16H20O4										-852.3	SWS	-752.7	-99.6
1,2-Benzenedicarboxylic acid dibutyl ester (Dibutyl o-phthalate)	C16H22O4 (1)	84-74-2	-750.9		-772.4	21.5	-842.6		-861.3	18.7				
Nonanedioic acid dibutyl ester	C17H32O4 (1)	2917-73-9					-1177.8		-1137.6	-40.2				
1,2,3-Propanetriol 1-tetradecanoate	C17H34O4 (1)	589-68-4									-1222.6		-1222.6	-0.0
1,2,3-Propanetriol 2-tetradecanoate	C17H34O4 (2)	3443-83-2									-1212.9		-1222.6	9.7
Bis(1-oxo-3-phenyl-2-propenyl)peroxide (Dicinnamoyl peroxide)	C18H14O4 (1)	15036-31-4									-356.1		-268.6	-87.5
1,2-Benzenedicarboxylic acid dipentyl ester	C18H26O4 (1)	131-18-0	-817.6		-814.2	-3.4	-924.3		-912.4	-11.9				
1,2-Benzenedicarboxylic acid bis-(3-methylbutyl)-ester	C18H26O4 (2)	605-50-5					-941.0		-925.8	-15.2				
(Z)-1,2-Cyclopentylene dibenzoate	C19H18O4										-667.3	SWS	-704.2	36.8
(E)-1,2-Cyclopentylene dibenzoate	C19H18O4										-674.9	SWS	-705.4	30.5
1,2,3-Propanetriol 1-hexadecanoyl ester (Glycerol a-palmitate)	C19H38O4 (1)	542-44-9									-1281.5		-1281.1	-0.4
1,2,3-Propanetriol 2-hexadecanoyl ester	C19H38O4 (2)	23470-00-0									-1268.7		-1281.1	12.4
1,2-Benzenedicarboxylic acid diphenyl ester	C20H14O4 (1)	84-62-8									-489.2		-491.6	2.4
(Z)-1,2-Cyclohexylene dibenzoate	C20H20O4										-718.4	SWS	-734.6	16.2

Table 6. Carbon-Hydrogen-Oxygen compounds (CxHyO3): Enthalpy of formation (298 K), 7

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
(E)-1,2-Cyclohexylene dibenzoate	C20H2004										-734.3	SWS	-734.7	0.4
(E)-1-Methyl-1,2-cyclopentylene dibenzoate	C20H2004										-702.9	SWS	-766.9	64.0
1,2-Benzenedicarboxylic acid dicyclohexyl ester	C20H2604 (1)	84-61-7									-931.4		-922.6	-8.8
(E)-1-Methyl-1,2-cyclohexylene dibenzoate	C21H2204						-759.0	SWS	-770.3	11.3				
1,2,3-Propanetriol 1-octadecanoyl ester	C21H4204 (1)	123-94-4									-1337.4		-1339.7	2.3
1,2,3-Propanetriol 2-octadecanoyl ester	C21H4204 (2)	621-61-4									-1321.3		-1339.7	18.4
(Z)-1,2-Indanylene dibenzoate	C23H1804										-555.2	SWS	-493.7	-61.5
(E)-1,2-Indanylene dibenzoate	C23H1804										-546.8	SWS	-496.2	-50.6
(Z)-1,2,3,4-Tetrahydro-2,3-naphthalene dibenzoate	C24H2004										-596.6	SWS	-558.1	-38.5
(E)-1,2,3,4-Tetrahydro-2,3-naphthalene dibenzoate	C24H2004										-587.0	SWS	-558.1	-28.9
(Z)-1,2,3,4-Tetrahydro-1,2-naphthalene dibenzoate	C24H2004										-596.2	SWS	-558.1	-38.1
(Z)-1,2,3,4-Tetrahydronaphthalene-1,2- dibenzoate	C24H2004										-589.9	SWS	-558.1	-31.8
1,2-Benzenedicarboxylic acid bis-(1-ethylhexyl) ester	C24H3804 (1)	15495-94-0					-1084.1		-1093.9	9.8				
2-Oxopentanedioic acid (2-Oxoglutaric acid)	C5H6O5 (1)	328-50-7									-1026.2		-1026.3	0.1
a-d-Xylose	C5H10O5 (1)	31178-70-8									-1057.8		-1060.6	2.8
d-Ribose	C5H10O5 (2)	50-69-1									-1047.3	P94	-1036.4	-10.9
1,3,5,7,9-pentaoxecane	C5H10O5 (3)	16528-92-0	-779.8		-790.4	10.6					-867.7		-868.2	0.5
d-Arabinose	C5H10O5 (4)	10323-20-3									-1057.9		-1060.6	2.7
Xylitol	C5H12O5 (1)	87-99-0									-1118.5		-1100.4	-18.1
1,2-Anhydro-3,4,5,6-alloinositol (Epoxyconduritol)	C6H10O5 (1)	23559-36-6									-906.2		-906.3	0.1
1,2,3-Propanetriol diacetate (Diacetin)'	C7H12O5 (1)	25395-31-7					-1120.7		-1084.1	-36.6				
Tetraethylene glycol	C8H18O5 (1)	112-60-7	-883.0		-887.0	4.0	-981.7		-1000.4	18.7				
3,5,7,9,11-Pentaoxatridecane	C8H18O5 (2)	5729-59-9	-905.9		-925.5	19.6	-968.4		-976.1	7.7				
2-(Diacetoxymethyl)furan	C9H10O5 (1)	613-75-2	-772.5		-772.4	-0.1					-882.1		-881.9	-0.2
(E)-4-tert-Butoxy-4-oxo-2-buteneperoxoic acid methyl ester	C9H14O5 (1)	49681-66-5					-746.7		-773.6	26.9				
4-tert-Butoxy-4-oxobutaneperoxoic acid methyl ester	C9H16O5 (1)	49681-67-6					-878.2		-879.1	0.9				
1,4,7,10,13-Pentaoxacyclopentadecare	C10H20O5 (1)	33100-27-5	-799.5		-799.6	0.1	-879.1		-879.1	-0.0				
Benzoylcarboxyperoxide phenyl ester	C14H10O5 (1)	962-16-3	-387.0		-425.1	38.1					-484.9		-506.7	21.8
Benzoyl(cyclchexyloxy)-carbonylperoxide	C14H16O5 (1)	20666-86-8	-645.3		-648.9	3.6					-741.5		-722.2	-19.3
Benzo-15-crown-5-ether	C14H20O5 (1)		-745.6	P94	-745.6	-0.0								
Tartaric acid, d	C4H6O6										-1256.9	SWS	-1286.9	30.0
Tartaric acid, meso	C4H6O6										-1259.4	SWS	-1286.9	27.5
Tartaric acid, d,l (racemic)	C4H6O6										-1278.2	SWS	-1286.9	8.7
Acetylenedicarboxylic acid dihydrate	C4H6O6										-1103.7	SWS	-1103.7	
(E)-1-Propene-1,2,3-tricarboxylic acid	C6H6O6 (1)	4023-65-8									-1232.7		-1250.6	17.9
(Z)-1-Propene-1,2,3-tricarboxylic acid	C6H6O6 (2)	585-84-2									-1224.4		-1246.4	22.0

Table 6. Carbon-Hydrogen-Oxygen compounds (CxHyO3): Enthalpy of formation (298 K), 8

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ
l-Ascorbic acid	C6H8O6 (1)	50-81-7									-1164.6		-1164.4	-0.2
Dimethyl tartrate, meso	C6H10O6										-1197.9	SWS	-1199.0	1.1
Dimethyl tartrate, d	C6H10O6										-1197.0	SWS	-1199.0	2.0
Dimethyl tratrate, racemic	C6H10O6										-1202.9	SWS	-1199.0	-3.9
a-D-Glucose	C6H12O6 (1)	26655-34-5									-1273.3		-1274.0	0.7
l-Sorbose	C6H12O6 (2)	87-79-6									-1271.5		-1271.5	0.0
b-d-Fructose (Pyranose form)	C6H12O6 (3)	57-48-7									-1265.6		-1290.8	25.2
b-d-Fructose (Furanose form)	C6H12O6 (3)	57-48-7									-1265.6		-1266.5	0.9
d-Mannose	C6H12O6 (4)	3458-28-4									-1263.0		-1274.0	11.0
a-d-Galactose	C6H12O6 (5)	3646-73-9									-1286.3		-1274.0	-12.3
b-Levulose, d	C6H12O6										-1269.8	SWS	-1266.5	-3.3
d-Mannitol	C6H14O6 (1)	87-78-5									-1337.1		-1313.8	-23.3
Galactitol (Dulcitol)	C6H14O6										-1346.8	SWS	-1313.7	-33.2
1,2,3-Benzene tricarboxylic acid	C9H6O6 (1)	569-51-7									-1160.3		-1156.5	-3.8
1,2,4-Benzene tricarboxylic acid	C9H6O6 (2)	528-44-9									-1179.1		-1182.0	2.9
1,3,5-Benzene tricarboxylic acid	C9H6O6 (3)	554-95-0									-1190.1		-1207.5	17.4
1,2,3-Propanetriol triacetate (Triacetin)	C9H14O6 (1)	102-76-1	-1245.2	P94	-1206.2	-38.9	-1330.9	P94	-1287.8	-43.1				
18-Crown-6-ether	C12H24O6 (1)										-1037.0	P94	-878.6	-158.4
Dibenzo-18-crown-6-ether	C26H24O6 (1)										-787.7	P94	-882.0	94.3
Citric acid	C6H8O7										-1543.9	SWS	-1567.7	23.8
Glucose hydrate	C6H14O7										-1572.3	SWS	-1585.7	13.4
Dipentaerythritol	C10H22O7										-1574.0	SWS	-1539.4	-34.6
1,2,3,4-Benzene tetracarboxylic acid	C10H6O8 (1)	476-73-3									-1548.6		-1546.0	-2.6
1,2,3,5-Benzene tetracarboxylic acid	C10H6O8 (2)	479-47-0									-1562.3		-1571.5	9.2
1,2,4,5-Benzene tetracarboxylic acid (Pyromellitic acid)	C10H6O8 (3)	89-05-4									-1570.8		-1571.5	0.7
1,2,4,5-Benzene tetracarboxylic acid tetraethyl ester	C18H22O8 (1)	6634-01-1									-1579.6		-1533.0	-46.6
1,2,4,5-Benzene tetracarboxylic acid tetrapropyl ester	C22H30O8 (1)	3143-08-6					-1649.1		-1669.8	20.7				
Pyromellitic acid tetrabutyl ester	C26H38O8 (1)	2451-79-8					-1752.5		-1771.8	19.3				
Benzenepentacarboxylic acid	C11H16O10 (1)	1585-40-6									-1929.7		-1935.5	5.8
Benzenepentacarboxylic acid pentamethyl ester	C16H16O10 (1)	3327-06-8									-1788.1		-1782.8	-5.3
d-Sucrose	C12H22O11 (1)	57-50-1									-2226.1		-2226.7	0.6
b-Lactose	C12H22O11 (2)	5965-66-2									-2236.7		-2234.3	-2.4
a-d-Glucose 2,3,4,5,6-pentaacetate	C16H22O11 (1)	3891-59-6**									-2249.4	#	-2102.5	-146.9
b-d-Glucose 2,3,4,5,6-pentaacetate	C16H22O11 (2)										-2232.6	#	-2102.5	-130.1
Benzenehexacarboxylic acid	C12H6O12 (1)	517-60-2									-2298.7		-2299.5	0.8
b-Maltose monohydrate	C12H24O12 (1)	6363-53-7									-2459.6		-2526.0	66.4
a-Lactose monohydrate	C12H24O12 (2)	10639-26-6									-2484.1		-2526.0	41.9
Benzenehexacarboxylic acid hexamethyl ester	C18H18O12 (1)	6237-59-8									-2110.8		-2116.3	5.5

Table 6. Carbon-Hydrogen-Oxygen compounds (CxHyO3): Enthalpy of formation (298 K), 9

Compound	Formula (PNK #)	CAS Registry No.	Gas				Liquid				Solid			
			Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ	Expt.	Ref.	Calc.	Δ

Notes and References

* Mixture of 1,2 diacetate [102-62-5] and 1,3-diacetate [105-70-4]
** May be [68069-84-1]
a: This value derived from C9H8O4(c) + H2O(l) = C2H4O2(lq1) + C7H6O3(c2); using the experimental value for C2H4O2(lq1) tabulated here, a value of -189.2 kcal/mol (instead of -194.9) is obtained.
These two values are from the same source (44CLA/STE) and are suspiciously low.

DH: E. S. Domalski and E. D. Hearing, "Estimation of Thermodynamic Properties of C-H-N-O-S-Halogen Compounds at 298.15 K," J. Phys. Chem. Ref. Data 22, 805 (1993).
S: S. E. Stein, J. M. Rukkers, and R. L. Brown, "NIST Structures & Properties Database and Estimation Program, NIST-SRD DB 25," Version 2.0 (1994).
P94: J. B. Pedley, "Thermochemical Data and Structures of Organic Compounds, Vol. 1" (TRC Data Series, 1994).
SWS: D. S. Stull, E. F. Westrum, Jr., and G. C. Sinke, "The Chemical Thermodynamics of Organic Compounds" (Krieger, 1987).

4. Acknowledgments

This work was carried out under Contract No. 43NANB420595 of the National Institute of Standards and Technology, whose support is gratefully acknowledged. The continued interest and advice of Professor S. W. Benson is also deeply appreciated. The painstakingly thorough evaluations of the two anonymous referees proved most helpful; their services considerably improved the paper.

5. References

[1] See S. W. Benson, *Thermochemical Kinetics*, 2nd ed. (Wiley, New York, 1976), and the references cited therein.

[2] F. D. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, *Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, Comprising the Tables of the American Petroleum Institute Research Project 44 Extant as of December 31, 1952* (Carnegie Press, Pittsburgh, 1953).

[3] D. R. Stull, E. G. Westrum, Jr., and G. C. Sinke, *The Chemical Thermodynamics of Organic Compounds* (Krieger, Malabar, FL, 1987).

[4] J. D. Cox and G. Pilcher, *Thermochemistry of Organic and Organometallic Compounds* (Academic, London, 1970).

[5] J. B. Pedley, R. D. Naylor, and S. P. Kirby, *Thermochemical Data of Organic Compounds*, 2nd ed. (Chapman and Hall, London, 1986).

[6] Pedley has recently revised the compilation of Pedley, Naylor, and Kirby in *Thermochemical Data and Structures of Organic Compounds* (Thermodynamics Research Center, Texas A&M University, 1994), Vol. 1.

[7] S. E. Stein, J. M. Rukkers, and R. L. Brown, NIST Structures & Properties Database and Estimation Program, NIST-SRD 25, Version 2.0 (1994).

[8] N. Cohen, Aerospace Corp. Report No. ATR-94(7263)-1, April 1994.

[9] K. Fajans, Chem. Ber. **53**, 643 (1920); **55**, 2826 (1922); M. S. Kharasch, J. Res. Natl. Bur. Stand. **2**, 359 (1929).

[10] S. W. Benson and J. H. Buss, J. Chem. Phys. **29**, 546 (1958).

[11] For a recent resume of the theory, see N. Cohen and S. W. Benson, in *The Chemistry of Alkanes and Cycloalkanes*, edited by S. Patai and Z. Rappoport (Wiley, New York, 1992), Chap. 6.

[12] Reference 1, p. 26.

[13] N. Cohen and S. W. Benson, Chem. Rev. **93**, 2419 (1993).

[14] S. G. Lias, J. E. Bartmess, J. F. Liebman, J. L. Holmes, R. D. Levin, and W. G. Mallard, J. Phys. Chem. Ref. Data **17**, Suppl. 1 (1988).

[15] E. S. Domalski and E. D. Hearing, J. Phys. Chem. Ref. Data **22**, 805 (1993).

[16] M. S. Kharasch, J. Res. Natl. Bur. Stand. **2**, 359 (1929).

[17] Particular mention should be made of an unpublished supplement, kindly supplied by S. W. Benson, to H. K. Eigenmann, D. M. Golden, and S. W. Benson, J. Phys. Chem. **77**, 1687 (1973), which contained references to a number of measurements not reported in other compilations.

[18] N. Cohen, Aerospace Corp. Report No. ATR-93(7263)-2, 1993.

[19] P. S. Nangia and S. W. Benson, J. Phys. Chem. **83**, 1138 (1979).

[20] L. G. S. Shum and S. W. Benson, Int. J. Chem. Kinet. **15**, 323 (1983); S. P. Heneghan and S. W. Benson, *ibid.* **15**, 815 (1983); O. Kondo and S. W. Benson, J. Phys. Chem. **88**, 6675 (1984); S. W. Benson and N. Cohen (unpublished).

[21] W. V. Steele, R. D. Chirico, A. Nguyen, I. A. Hossenlopp, and N. K. Smith, in *Results from the Design Institute for Physical Property Data: Experimental Results and Data Compilation Procedures*, edited by J. R. Cunningham and D. K. Jones (AIChE Symposium Series, New York, 1990), Vol. 86, No. 279, pp. 138–154.

[22] See, for example, Y. G. Wu, S. N. Patel, E. R. Ritter, and J. W. Bozzelli, Thermochim. Acta **222**, 153 (1993).

[23] H. K. Eigenmann, D. M. Golden, and S. W. Benson, J. Phys. Chem. **77**, 1687 (1973).

[24] Problematic compounds are discussed in more detail in Ref. 18 and in N. Cohen, Thermochemical Kinetics Research Report No. TKR 95-1, 1995.