Estimation of the Thermodynamic Properties of C-H-N-O-S-Halogen Compounds at 298.15 K

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Estimation of the Thermodynamic Properties of C-H-N-O-S-Halogen Compounds at 298.15 K

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An estimation method, which was developed by S.W. Benson and coworkers for calculating the thermodynamic properties of organic compounds in the gas phase, has been extended to the liquid and solid phases for organic compounds at 298.15 K and 101,325 Pa. As with a previous paper dealing with hydrocarbon compounds, comparisons of estimated enthalpies of formation, heat capacities, and entropies with literature values show that extension of the Benson's group additivity approach to the condensed phase is easy to apply and gives satisfactory agreement. Corresponding values for the entropy of formation, Gibbs energy of formation and natural logarithm of the equilibrium constant for the formation reaction are also calculated provided necessary auxiliary data are available. This work covers 1512 compounds containing the elements: carbon, hydrogen, oxygen, nitrogen, sulfur, and halogens in the gas, liquid, and solid phases. About 1000 references are provided for the literature values which are cited.

Keywords: enthalpy of formation; entropy; estimation; heat capacity; organic compounds; thermodynamic properties.

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1. Introduction

The purpose of this paper is to demonstrate that the estimation of thermodynamic properties of organic compounds in the condensed phase at 298.15 K and 101,325 Pa can be carried out in a satisfactory manner using established second-order group-additivity methods. The second-order group-additivity method, originally introduced by S.W. Benson and coworkers (58BEN/BUS, 68BEN, 69BEN/CRU, 69SHA, 71SHA, 73EIG/GOL, 76BEN, 77LUR/BEN, 77SHA/GOL, 77STE/GOL) for estimating the thermodynamic properties of organic compounds, was developed and used primarily for the gas phase. This work includes a re-examination of the capabilities for estimation of the thermodynamic properties of the gas phase to maintain continuity with the condensed phase and also to introduce changes in group values necessitated by more recent thermodynamic data available in the literature.

The coverage of organic compounds includes those substances containing the elements: carbon, C; hydrogen, H; oxygen, O; nitrogen, N; sulfur, S; fluorine, F; chlorine Cl; bromine, Br; and iodine, I. The particular thermodynamic properties for which groups and group values have been determined are: enthalpy of formation, $\Delta_t H^\circ$; heat capacity, C_p° ; and entropy, S° . The entropy of formation $(\Delta_t S^\circ)$, Gibbs energy of formation $(\Delta_t G^\circ)$, and the natural logarithm of the equilibrium constant (ln K_t) for the formation reaction, are calculated as auxiliary properties.

The second-order group-additivity approach has been generally accepted by physical chemists and chemical engineers because of the simple basis of additivity, clarity of notation, second-order character, i.e., inclusion of nearest-neighbor interactions, ease of application, and satisfactory agreement between the thermodynamic value reported in the literature and its estimated value. The ASTM Chemical Thermodynamic and Energy Release Program, CHETAH, (74SEA/FRE)) uses these methods for the estimation of the thermodynamic properties of organic compounds in the gas phase and for the classifi-

cation of chemicals or compositions depending upon whether they are likely to be impact sensitive. The AIChE Design Institute for Physical Property Data (DIPPR) Manual for Predicting Chemical Process Design Data (83DAN/DAU) recommends the second-order group-additivity method (76BEN) for the estimation of enthalpy of formation, heat capacity, and entropy of organic compounds at 298.15 K in the gas phase. DIPPR Project 871 is an experimental project begun to determine accurate enthalpies of formation and vaporization of key organic compounds so that reliable gas phase enthalpies of formation can be calculated at 298.15 K. The latter data would then permit either the calculation of new second-order group-additivity values or the replacement of group values which are based on poor quality data. The improved or new group values would be used to upgrade both the DIPPR Data Prediction Manual and the ASTM CHETAH Program.

With such broad needs for thermodynamic property estimation in ASTM and AIChE, we felt that the successful application of this approach for the gas phase merited an intensive examination of its application into the condensed phase. The approach taken for the evaluation of thermodynamic data and the path of development of groups and group values for hydrocarbon compounds came from our previous paper (88DOM/HEA) in which a systematic procedure was followed for the selection of group values which gave minimum residuals between the literature and calculated values. The n-alkanes from C₂ to C₁₈ make up one of the most studied families of compounds and have some of the most pristine values for $\Delta_t H^{\circ}$, C_p° , and S° of all the families of organic compounds. They form the basis for the development of the $C-(H)_3(C)$ and $C-(H)_2(C)_2$ group values. From this point, the group and group value development proceeds to branched alkanes, alkenes, alkynes, aromatic and alicyclic compounds, CHO compounds (alcohols, ethers, etc.), CHN compounds (amines, nitriles, etc.), and on to CHNO, CHS, CHSO, and organic halogen compounds. Care is needed in the development of group values because experimental or recommended data have different degrees of quality and are not homogeneous. Reduction of data to as common a basis as possible is required. For combustion data, some previously established guidelines were used (71DOM). A global least squares, least sums, or regression-type fit of all the group values was not performed because of the differences in the quality of the data, and because of the limited amount of data available for the generation of certain groups and group values. The generation of groups and the calculation of group values was in part manual and in part computerassisted. Some computations for average values, average deviations, or standard deviation were performed using a desk-top calculator. Others were made using computer spread-sheet analysis.

The group values generated for the hydrocarbons were held fixed for the generation of non-hydrocarbon values. Most of the group values for non-hydrocarbon compounds were generated using the THERM/EST Program

(NIST Standard Reference Database 18) (90DOM/ HEA2) by having the group value being sought initially become part of the residual value. In this procedure, an unknown group value is calculated, then a value is assigned to the unknown group, and a final or true residual value is calculated which excludes the new group value, but minimizes the final residual value. When a large number of experimental values were available to calculate a group value, as with n-alkanes, n-alkanols or n-alkanethiols, final adjustments were examined with computer spread-sheet software. Care was taken to accommodate the adjusted group values when the same groups were needed for different families of compounds. For example, the $C-(H)_2(C)(O)$ group and its group values are required for alcohols, ethers, esters, and peroxides. Group values for some families or compounds were generated simply by calculating simple arithmetic averages because the experimental data were limited to 2 or 3 values. The group C-(H)₃(C) is used freely in the molecular structure representation of compounds because the value of the methyl group does not change except for the physical phase no matter to what it is attached. Hence, $C-(H)_3(C) = C-(H)_3(O) = C-(H)_3(N)$ = $C-(H)_3(S)$, etc., and consequently, methanol can be represented by: $C-(H)_3(C) + O-(H)(C)$ rather than: $C-(H)_3(O) + O-(H)(C)$. Appendix 1 lists unique groups derived from data on individual compounds as their

The compounds for which estimated properties have been calculated are divided into various organic families as shown in Table 1. The number of compounds within each family is indicated. A total of 1512 compounds have had thermodynamic properties estimated and compared with a literature value. This total is not exhaustive, but does represent a sufficiently broad array of organic structures to demonstrate the applicability of the group additivity method to the condensed phase. Compounds are listed according to the increasing number of carbon atoms within each family, but sometimes the carbon number reverts back to lower values because of the inclusion of certain compounds with secondary or tertiary substitution, unsaturation, multiple functional groups, aromatic substitution, or cyclic structures. Table 2 provides a listing of over 600 groups and energy corrections. and their corresponding values for $\Delta_t H^{\circ}$, C_n° , and S° for the gas, liquid, and solid phases. Table 3 offers some guidance to the definition and interpretation of organic groups for persons not accustomed to the notation in Table 2.

Thermodynamic properties for 1512 compounds are shown in Tables 4 through 54 and contain the following information: the title of the organic family, the number of compounds included in that family, individual compound name(s), formula of the compound, the organic groups which comprise the structure of the compound, symmetry number, σ , and optical isomers, η . Thereafter, each phase is treated separately, gas, liquid, and solid. Property symbols $\Delta_t H^{\circ}$ (in kJ/mol), C_p° (in J/mol·K), and S° (in J/mol·K) appear in the extreme left column. Next, the ex-

perimental or recommended values are also given, when available, and entered under the column, "Literature". The property value derived from summing the group values is given under the column, "Calculated", so that a difference or residual value may be calculated and shown under the column, "Residual". The residual offers an indication of how close the estimated value comes to the one determined experimentally or to the one derived from an evaluation of a collection of literature data. If the appropriate group values are available so that the enthalpy of formation and entropy can be estimated, we also provide the entropy of formation, $\Delta_f S^{\circ}$ (in J/mol·K), Gibbs energy of formation, $\Delta_f G^{\circ}$ (in kJ·mol⁻¹), and the logarithm of the equilibrium constant for the formation process, lnK_f. In order to calculate the entropies of formation at 298.15 K and 101,325 Pa, the entropies of the elements in their standard states are needed as well as the entropies of the respective compounds. The entropies of the elements at 298.15 K and at 101,325 Pa have been obtained from (89COX/WAG) and are as follows in J/ mol·K: carbon (cr,graphite), 5.740; H₂ (gas), 130.571; O₂ (gas), 205.043; N₂ (gas), 191.500; S (cr, rhombic), 32.054; F₂ (gas), 202.682; Cl₂ (gas), 222.972; Br₂ (liquid), 152.21; I_2 (cr), 116.14. Estimation of the entropy in the gas phase requires a $-R \ln \sigma$ term where σ is the total symmetry number of the molecule and R is the universal gas constant (R = 8.31451 J/mol·K). The total symmetry number of the molecule is divided into two parts: the internal symmetry number and the external symmetry number. The definitions of the latter symmetry numbers and several example calculations of symmetry numbers can be found in (88DOM/HEA). Estimation of the gas phase entropy also requires accounting for optical isomers as the molecular structure dictates with a Rln η term, where η indicates the number of such isomers. Since this work deals with data at only one temperature, 298.15 K, no distinction is made between the heat capacity at constant pressure, C_p° , and the saturation heat capacity, C_{sat} .

Reference squibs appear in the extreme right column of the tables under the heading "References"; The squibs are of the type XXAAA/BBBN for each property in each of the phases and correspond to entries under the column "Literature". In this squib notation, XX denotes the last two digits of the year of publication of the paper, AAA, the first three letters of the last name of the first author, and BBB, those of the last name of the second author (if present). Authors after the first two are not noted. The numeral, N, at the end of the squib is present only when the authors have more than one paper published in a given year. Table 55 provides a summary of the residuals for each family which offers some global insight into the agreement realized between literature and calculated values. The residuals have been divided into those for $\Delta_t H^{\circ}$ which were $\langle \pm 4, \rangle \pm 4$ but $\langle \pm 8, \text{ and } \rangle \pm 8 \text{ kJ·mol}^{-1}$. Similarly, for C_p° and S° , the residuals have been divided into those which were $< \pm 4$, $> \pm 4$ but $< \pm 8$, and $> \pm 8$ J/mol·K. Table 56 shows an alphabetical compound name-formula index which provides the CAS registry number, family in which the compounds may be found, its

listing or rank within the given family, and the page on which data for the compound appears. A bibliography given in Table 57 with about 1000 references links reference squibs in Tables 4 through 54 to literature citations.

We have examined the original reference sources for data on the enthalpies of formation, heat capacities, and entropies for almost all of the compounds. The thermodynamic tables compiled by Stull, Westrum, and Sinke (69STU/WES, 69STU/WES2) have been used for many of the literature gas phase heat capacities and entropies. We have also used some general thermodynamic reference sources to find original sources in certain cases (70COX/PIL, 71ZWO/WIL, 72DOM, 77PED/RYL, 84DOM/EVA, 85MAJ/SVO, 86TRC, 86TRC2, 86PED/NAY, 90DOM/HEA). Over 3700 comparisons between literature and calculated values are shown for $\Delta_t H^\circ$, C_p° , and S° in the gas, liquid, and solid phases. Approximately half of the comparisons are for the condensed phase.

Interpretation is occasionally required when a reference squib is designated for a specific property. For example, a reference squib denoted for $\Delta_t H^{\circ}$ in the gas phase may not actually provide that specific property, but will report an enthalpy of vaporization at 298.15 K which when added to $\Delta_i H^\circ$ in the liquid phase, will then be equal to the designated experimental or recommended $\Delta_f H^{\circ}$ (gas) value. Similarly, a reference squib denoted for $\Delta_i H^{\circ}$ (solid) may not contain the actual $\Delta_i H^{\circ}$ property for the solid phase, but does report the ΔH° for the fusion or melting of the compound. When the latter is corrected from the melting temperature to 298.15 K and combined with $\Delta_i H^{\circ}(\text{liq})$ at 298.15 K, one obtains the $\Delta_i H^{\circ}(\text{solid})$ value. Despite concerns related to the estimation of thermodynamic properties for solid substances, we typically find good agreement between literature and calculated values. Common doubts about the ability to develop a predictive scheme for solid substances arise because some organic compounds have many crystalline forms in the proximity of the melting point. The second-order group-additivity approach does have its limits. We expect that the predicted solid phase at 298.15 K is the same as the stable form encountered experimentally at 298.15 K. For organic compounds with multiple crystalline phases and solid-solid transitions, as found with the C_{13} , C_{14} , and C₁₅ 1-alkanols, the group additivity approach provides only a limited value for the thermodynamic property. We do not feel that this limitation diminishes the overall usefulness of prediction of this method for solid organic substances. Appendix 2 shows that internal consistency does exist when comparisons are made between literature values for enthalpies and entropies of fusion and enthalpies of vaporization and the estimated differences for $[\Delta_i H^{\circ}(\text{solid}) - \Delta_i H^{\circ}(\text{liq})], [S^{\circ}(\text{solid}) - S^{\circ}(\text{liq})], \text{ and}$ $[\Delta_i H^{\circ}(\text{liq}) - \Delta_i H^{\circ}(g)]$, at 298.15 K. Differences between literature values for enthalpies and entropies of fusion corrected from the melting temperature to 298.15 K and $[\Delta_i H^{\circ}(\text{solid}) - \Delta_i H^{\circ}(\text{liq})]$ and $[S^{\circ}(\text{solid}) - S^{\circ}(\text{liq})]$ yield average deviations of $\pm 2.7 \text{ kJ.mol}^{-1}$ and $\pm 4.7 \text{ J/mol} \cdot \text{K}$, respectively. A similar comparison between literature values for the enthalpy of vaporization corrected to 298.15 K and $[\Delta_i H^{\circ}(\text{liq}) - \Delta_i H^{\circ}(g)]$ gives an average deviation of $\pm 1.6 \text{ kJ·mol}^{-1}$.

The quality of the groups and group values can be evaluated by examining the magnitude of the difference (or residual) which is observed between the literature and calculated values for a specific property in a given physical phase. For $\Delta_i H^\circ$, differences within ± 4 kJ/mol constitutes very good or satisfactory agreement, those which are between ±4 and ±8 kJ/mol are at the limits of acceptability, and differences which are greater than ±8 kJ/mol are symptomatic of a problem. The occurrence of differences larger than ±8 kJ/mol are usually due to poor quality literature data or to a neglected molecular interaction, both of which can lead to the incorrect assignment for a group value. A similar situation applies to heat capacity and entropy differences. When differences within ±4 J/mol·K occur, the agreement is considered very good, when they are between ± 4 and ± 8 J/mol·K, the agreement is acceptable, and when the differences are greater than ±8 J/mol·K, they reflect a problem, which similarly can be related to poor quality data or to a neglected molecular interaction, and can lead to the selection of an incorrect group value.

Certain molecules such as methane, methanal, acetonitrile, nitromethane, and the methyl halides are precluded from the rules of group additivity because they are structurally comprised of only one group and, hence, their group value is equivalent to the corresponding property value in each of the phases. We have included a number of such substances at the beginning of some of the organic families for comparison purposes. When needed for various calculations, the 1989 table of atomic weights was used (91DEL/HEU).

2. Discussion of Results

2.1. Hydrocarbon Compounds

The hydrocarbon compounds and thermodynamic properties appearing in 88DOM/HEA are also presented here as well as the calculation of the entropy of formation, Gibbs energy of formation, and equilibrium constant for the formation reaction. A total of 48 hydrocarbon compounds has been added which have created more groups and group values. A small number of groups and group values appearing in 88DOM/HEA have also been modified. Hydrocarbons comprise the most studied single famly of organic compounds from a thermodynamic standpoint and form the foundation for the development of groups and group values not only within hydrocarbons themselves but also for non-hydrocarbon compounds. Thermodynamic property comparisons between hydrocarbons and non-hydrocarbons permit one to test whether additivity is being preserved, whether molecular forces are interacting, or whether the literature values may be suspect.

The hydrocarbon compounds examined have been divided into eleven families: *n*-alkanes, *t*-alkanes, *q*-alkanes, *n*-alkenes, *s*-alkenes, alkynes, aromatic

CH-01, aromatic CH-02, cyclic CH-01, cyclic CH-02, and cyclic CH-03. These families contain thermodynamic property estimates for a total of 427 hydrocarbon compounds and are found in Tables 4 through 14. An examination of the 532 comparisons between literature and calculated values for $\Delta_i H^\circ$ shows that 70 percent of the residuals are $<\pm 4$ kJ/mol, 17 percent are $>\pm 8$ kJ/mol. For C_p° with 361 comparisons, we find 85 percent of the residuals $<\pm 4$ J/mol·K, 8 percent $>\pm 4$ but $<\pm 8$ J/mol·K, and 7 percent $>\pm 8$ J/mol·K. Similarly, for S° with 338 comparisons, we find 76 percent of the residuals $<\pm 4$ J/mol·K, 16 percent $>\pm 4$ but $<\pm 8$ J/mol·K, and 8 percent $>\pm 8$ J/mol·K, 16 percent $>\pm 4$ but $<\pm 8$ J/mol·K, and 8 percent $>\pm 8$ J/mol·K.

A novel approach for dealing with branched alkanes has been described in (88DOM/HEA) for tertiary and quaternary carbon atoms in hydrocarbon compounds. It corrects for the repulsive interactions of hydrogen atoms on methyl groups attached to tertiary or quaternary carbon atoms and improves the agreement between literature and estimated values. The corrections for methyl repulsion in branched hydrocarbons have been developed only for $\Delta_t H^\circ$ at 298.15 K. It accommodates the observation that as branching increases for an isomeric hydrocarbon, the $\Delta_t H^\circ$ value becomes more negative (e.g., $\Delta_t H^\circ$ s for isomeric pentanes). A summary of this approach can be found in (88DOM/HEA).

Except for n-hexacosane, residuals calculated from literature and calculated values for C_p° and S° for n-alkanes with carbon atoms C_{20} and higher are large, but do not come from recent calorimetric investigations. We suggest that some re-determination and confirmation is needed for the C_p° and S° values for these hydrocarbon compounds.

2.2. Organic Oxygen Compounds

After hydrocarbon compounds, organic oxygen compounds are the next most abundant category of organic substances for which thermodynamic data are available. The CHO compounds have been divided into 11 families: alcohols, ethers, aldehydes, ketones, acids, anhydrides, esters, peroxides, hydroperoxides, peroxyacids, and carbonates, and are found in Tables 15 through 25. These tables contain thermodynamic property estimates for 381 CHO compounds. An examination of 570 comparisons of literature and calculated values for $\Delta_i H^{\circ}$ shows that 62 percent have residuals which are $< \pm 4$ kJ/mol, 18 percent are $> \pm 4$ but $< \pm 8$ kJ/mol, and 20 percent are $> \pm 8$ kJ/mol. Residuals for C_p° show that 72 percent are $< \pm 4$ J/mol·K, 15 percent are between $> \pm 4$ and $< \pm 8$ J/mol·K, and 13 percent are $> \pm 8$ J/mol·K. For S°, 72 percent of the residuals are $< \pm 4$ J/mol·K, 16 percent are $> \pm 4$ but $< \pm 8$ J/mol·K, 12 percent are $> \pm 8$ J/mol·K.

Comparison of literature and calculated values for ΔH° , C_{p}° , and S° shows that for primary alcohols the agreement is reasonably good. However, initial agreement between literature and estimated values for secondary and tertiary alcohols was not as good as with

primary alcohols. We found that significantly smaller residuals resulted for secondary and tertiary alcohols if a methyl repulsion correction was applied for tertiary or quaternary carbon atom attached to an oxygen atom.

Agreement between literature and calculated values for secondary aliphatic alcohols, diols, triols, and tetrols for $\Delta_t H^\circ$, C_p° , and S° are somewhat inconsistent. Large residuals occasionally appear but do not seem to show a consistent trend. The residuals for some phenolic compounds can be improved with the application of an *ortho* correction for OH-OH interactions. Some of the literature data are not recent and may be suspect.

We found that better agreement between literature and calculated values was obtained if separate C-(H)(C)2(O) and C-(C)3(O) groups were assigned to alcohols and peroxides, and another for ethers and esters, rather than having global groups for all of the organic oxygen families. Hence, this separation is indicated in the list of groups and group values in Table 2 and under each compound in Tables 4 through 54 in the structural group notation.

Literature and calculated values for $\Delta_t H^\circ$, C_p° , and S° for ethers and ketones show generally good agreement. This is possible because of a significant quantity of good quality data in the gas and condensed phases.

For aldehydes, agreement between literature and calculated values for $\Delta_t H^{\circ}, C_p^{\circ}$, and S° in the gas phase are generally satisfactory. Although satisfactory agreement is found for $\Delta_t H^{\circ}(\text{liq})$, agreement for C_p° and S° in the liquid phase is poor. The C_p° and S° data of 56PAR/KEN at 298.15 K for butanal and heptanal in the liquid phase reflect the expected linear relationship when n-alkanals increase by a CH2 group. The recent data reported for ethanal by 88LEB/VAS, propanal by 77KOR/VAS, butanal by 89VAS/LEB, hexanal by 91VAS/BYK, and heptanal by 83DYA, 84VAS/PET indicate that the relationship for 1-alkanals in the liquid phase is neither linear nor smooth. These authors describe anomalies in the liquid phase which they have found to be due to association in 1-alkanals through hydrogen bonds. The group values we have chosen are based on linearity, hence, significant deviation are reflected in the large residuals which occur.

We have found some large differences between the literature and calculated values for $\Delta_t H^\circ$ and C_p° for dibasic acids in the gas and solid phases. It is not clear whether these residuals are due to hydrogen bonding in dibasic acids, odd-even carbon atom effects, the need for a group correction factor, poor experimental data, or most of the above. A significant amount of these data were reported in the 1920's. It may be possible that the odd-even relationship which is observed for the melting temperatures of dicarboxylic acids is similarly reflected in their thermodynamic properties. A large fraction of the residuals in $\Delta_t H^\circ$'s for the dibasic acids are $> \pm 8$ kJ/mol.

The experimental $\Delta_t H^\circ$ values for 1-naphthoic and 2-naphthoic acid differ from each other by 9.4 kJ/mol in the gas phase and 12.4 kJ/mol in the solid phase. Examination of the structures of these acids by 74COL/ROU indicates that 2-naphthoic acid is planar, but 1-naphthoic

acid is twisted 11° out of the naphthalene plane due to overcrowding, hence, these structural differences account for the observed energy differences.

Corrections have been developed for *ortho* and *meta* interactions between two or more carboxylic acid groups in aromatic acids. Similar corrections were developed for interactions between methoxy and carboxylic acid groups. In some instances, a clear interaction correction was not developed because the nature of the interaction between adjacent or near-adjacent groups could not be interpreted clearly, and/or the quality of the experimental data did not allow an interpretation. In these cases, we applied the *ortho* and *meta* corrections developed for hydrocarbon compounds.

Difficulty in resolving the agreement between literature and calculated $\Delta_t H^\circ$ values for benzoic anhydride with aliphatic anhydrides led to the development of separate groups for O-(CO)2 and corresponding attachments to aliphatic and aromatic substituents. They are listed in Table 2 as: O-(CO)2, aliphatic and O-(CO)2, aromatic.

Thermodynamic property data on peroxides, hydroperoxides, and peroxyacids are limited to enthalpies of formation. From time to time, agreement between $\Delta_t H^\circ$ experimental and calculated values is poor. This situation is due to a lack of high quality data on these substances and is understandable because of their explosive and thermally sensitive character. The preparation of sufficient amounts of high purity samples of thermally sensitive substances places a very high demand upon any research effort.

The unusually large difference between the literature and calculated $\Delta_i H^o$ for diacetyl peroxide (DAP) in the liquid phase (see Table 21, 38.66 kJ/mol) may be due to the instability of the compound. Because of its instability, bomb calorimetric experiments on diacetyl peroxide were performed on a toluene solution (37.53 wt% DAP, 62.47wt% toluene; 57JAF/PRO). Bomb calorimetric experiments were made at only one concentration of DAP in toluene, hence, dilution errors or analytical errors cannot be easily detected. Examination of the experimental and calculated values for dipropionyl and dibutyryl peroxides shows their residuals to be satisfactory.

The differences found between the literature and estimated values for peroxy acids are large. The groups developed for the family appears to be the best that can be assembled. If some re-determinations of the thermodynamic properties for peroxy acids can be made, smaller residuals may result.

2.3. Organic Nitrogen Compounds

Literature and estimated thermodynamic properties on organic nitrogen compounds have been divided in seven CHN families and nine CHNO familes. The families which comprise the CHN compounds are: amine, imines, nitriles, hydrazines, diazenes, azides, and cyclic CHN compounds and are found in Tables 26 through 32. A total of 137 CHN compounds are shown. Agreement between experimental and calculated values shows 84

percent of the residuals for $\Delta_t H^\circ$ to be $<\pm 4$ kJ/mol, 10 percent of the residuals for $\Delta_t H^\circ$ to be $<\pm 4$ kJ/mol, 10 percent are $>\pm 4$ but $<\pm 8$ kJ/mol, and 6 percent are $>\pm 8$ kJ/mol. For C_p° , 85 percent of the residuals are $<\pm 4$ J/mol·K, 7 percent are $>\pm 4$ but $<\pm 8$ J/mol·K, and 8 percent are $>\pm 8$ J/mol·K. With respect to S° , 77 percent of the residuals are $<\pm 4$ J/mol·K, 15 percent are $>\pm 4$ and $<\pm 8$ J/mol·K, and 4 percent are $>\pm 8$ J/mol·K.

The families which comprise the CHNO compounds are: amides, ureas, amino acids, nitroso, nitro, nitrites, nitrates, nitrates, nitramines, and cyclic CHNO compounds. A total of 171 CHNO compounds are shown in Tables 33 through 41. Comparison of literature and calculated values show that for $\Delta_t H^\circ$ residuals, 68 percent are $< \pm 4$ kJ/mol, 11 percent are $> \pm 4$ but $< \pm 8$ kJ/mol, and 21 percent are $> \pm 8$ percent. For C_p° , 80 percent of the residuals are $< \pm 4$ J/mol·K, 6 percent are $< \pm 4$ but $> \pm 8$ J/mol·K, and 14 percent are $> \pm 8$ J/mol·K. For S° , 69 percent are $< \pm 4$ J/mol·K, 10 percent are $< \pm 4$ but $> \pm 8$ J/mol·K, and 21 percent are $> \pm 8$ J/mol·K.

From an initial examination of the differences between the literature and calculated values, the CHN family appears to be amenable to prediction. We have applied the -CH₃ quaternary correction for alkane branching to nitrogen atoms in tertiary amines, N,N-dimethylsubstituted amides, and N,N-dimethylsubstituted ureas because better agreement resulted between experimental and estimated values. A corresponding application of the -CH₃ tertiary correction to nitrogen atoms in secondary amines, N-methylsubstituted amides, or N-methyl substituted ureas was not used because it did not lead to significantly smaller differences between experimental and estimated values.

Comparison of the experimental $\Delta_t H^\circ$ for the solid phase of acetamide with the estimated value shows a difference of -10.41 kJ/mol. This difference is larger than one would like. However, anomalous behavior has been reported for crystalline acetamide due to its tendency to supercool (86EMO/NAU). Acetamide forms an unstable solid phase along with a stable form. The stable and unstable forms have melting temperatures of 353.5 K and 342.15 K, and enthalpies of melting of 15.6 and 12.5-12.9 kJ/mol, respectively.

The estimation of the thermodynamic properties of amino acids and peptides in the solid phase is a particularly challenging task. Some amino acids have been the subject of a significant amount of calorimetric study; glycine and hippuric acid are examples. Other amino acids as well as peptides have received only limited calorimetric attention. There is a mixture of high quality, medium quality, and limited quality data on these compounds. Other challenges included accounting for the dipolar nature of amino acids, and identifying differences when possible between (DL) racemic and optically active (R or D, and S or L) isomers. Because the enthalpy of combustion and formation of glycine has been so frequently determined, we have used the experimental values for this amino acid and the corresponding data on

glycylglycine as the basis for deriving the C-(H)2(CO)(N) group and group value and the energy correction for the dipolar nature or zwitterion character of aliphatic amino acids. Since the zwitterion nature of amino acids and peptides is a unique property and not prominent in the other organic nitrogen compounds treated in this paper, a separate identification and energy correction was warranted. The establishment of the zwitterion energy correction also allows the C-(H)2(CO)(N) group to have property values not seriously divergent from those groups such as C-(H)2(C)2, C-(H)2(C)(CO), and C-(H)2(C)(N). The zwitterion energy correction for solid aliphatic amino acids and peptides for $\Delta_t H^\circ$, C_p° , and S° are -55.10kJ/mol, -44.50 J/mol·K, and -13.40 J/mol·K, respectively. Using similar reasoning, a zwitterion energy correction was developed for amino acids and peptides containing an aromatic ring, but required differentiation between situations in which a -CH₂- group breaks the conjugative nature of the aromatic ring from its linkage to the α -carbon of an amino acid or peptide. For these cases, the zwitterion energy is designated as "aromatic I" and was derived from $\Delta_i H^\circ$ (solid) data for phenylalanine and phenylalanine peptides; the zwitterion energy correction (for aromatic I) for $\Delta_i H^\circ$, C_p° , and S° are -32.00kJ/mol, -20.50 J/mol·K, and -13.00 J/mol·K, respectively. For situations in which the aromatic ring of an amino acid or peptide is bonded directly to amino groups or to carboxylic acid groups where the influence to ring conjugation should be stronger than it is for phenylalanine derivatives, a second aromatic zwitterion energy correction was derived to accommodate the estimation of the aminobenzoic acids, hippuric acid, and hippurylglycine, and designated as "aromatic II"; the zwitterion energy correction (for aromatic II) for $\Delta_t H^{\circ}$, C_p° , S° are -11.00 kJ/mol, 5.00 J/mol·K, and -9.00 J/mol·K, respectively. These group values are also found in Table 2. Agreement between literature and estimated values is variable. Future reconciliation of the large residuals may result from more precise calorimetric determinations of certain amino acids and peptides as well as some re-adjustment of group values. Better agreement was obtained between literature and estimated values when N-(H)2(CO) and N-(H)(C)(CO) groups were developed separately for amides and ureas in comparison to amino acids and peptides. At this time, it is not clear whether the better agreement is a function of differences in the molecular structure of these organic families or whether more accurate experimental data will offer new changes to their estimation.

The residual value for $\Delta_t H^\circ$ (solid) for nitrosobenzene is large, -85.65 kJ/mol. The group, CB-(NO), and corresponding $\Delta_t H^\circ$ group values, were derived from experimental data on 4-nitroso-1-naphthol. The $\Delta_t H^\circ$ experimental data for 4-nitroso-1-naphthol (68HAM/FAG) are more reliable than those for nitrosobenzene (30DRU/FLA). The large residual for nitrosobenzene is probably due to either sample purity or to difficulties with experimental bomb calorimetric procedures, or both.

As the development of the second-order group additivity approach to the estimation of thermodynamic properties (57BEN/BUS, 69BEN/CRU) began, the enthalpy of formation of the benzene (C_6H_6) molecule was divided by six to derive the group value for $\Delta_t H^{\circ} C_B - (H)(C_B)_2$ group in the gas phase. In this division, the resonance or conjugation energy of benzene (~150 kJ·mol⁻¹) had also undergone a corresponding division. We have attempted to extend this concept to pyridine and have introduced the N_{Γ} (C_B) group which not only includes the energy content for a property, but also the corresponding component of the conjugation energy which resides in the pyridine molecule. Reasonable success was achieved for pyridine and substituted pyridines in Table 32. The further extension of this concept to five-membered ring systems becomes a more difficult task when they possess an intrinsic and sizeable conjugation energy, but in addition, contain a significant amount of strain energy. This situation is true for five-membered systems such as furan, pyrrole, and thiophene. We have treated the carbon atoms in these five-membered ring systems as benzene carbon atoms, using the C_B-(H)(C_B)₂ group, because their conjugation energies are in the range from 65 to 120 kJ·mol⁻¹. As a result of this treatment, the $\Delta_i H^{\circ}$ ring strain corrections (rsc) for furan, pyrrole, and thiophene appear as negative values. In contrast, the conjugation energy in 1,3-cyclopentadiene is small when compared with its ring strain energy and its structural description has been assembled using C_d -(H)(C_d) and C_d -(H)(C) groups rather the $C_B-(H)(C_B)_2$ group.

2.4. Organic Sulfur Compounds

The families which comprise the CHS and CHSO compounds are: thiols, sulfides, disulfides, sulfoxides, sulfones, sulfites, sulfates, and cyclic CHS compounds. A total of 138 CHS and CHSO compounds are shown in Tables 42 through 49. Agreement between literature and calculated values shows 80 percent of the residuals for $\Delta_t H^\circ$ to be $<\pm 4$ kJ·mol⁻¹, 14 percent of the residuals to be $>\pm 4$ but $<\pm 8$ kJ·mol⁻¹, and 6 percent to be $>\pm 8$ kJ·mol⁻¹. For C_p° , 92 percent of the residuals are $<\pm 4$ J·mol⁻¹·K⁻¹, 7 percent are $>\pm 4$ but $<\pm 8$ J·mol⁻¹·K⁻¹, and 1 percent are $>\pm 8$ J·mol⁻¹·K⁻¹. For S° , 87 percent of the residuals are $<\pm 4$ J·mol⁻¹·K⁻¹, 7 percent are $>\pm 4$ but $<\pm 8$ J·mol⁻¹·K⁻¹, and 6 percent are $>\pm 8$ J·mol⁻¹·K⁻¹,

Excluding hydrocarbon compounds, organic sulfur compounds containing the elements C, H, and S stand out as offering an extremely high quality array of experimental thermodynamic values for $\Delta_t H^\circ$, C_p° , and S° . The establishment of this high quality array of data on CHS compounds is due to the need of the petroleum industry to understand the thermochemistry of organic sulfur compounds because of their presence in petroleum and because of the need to understand their energetics and equilibrium properties in petroleum refining. Much of the effort to establish high quality thermodynamic data for this class of organic compounds resulted from an ex-

perimental effort which took place at the U.S. Bureau of Mines Thermodynamics Laboratory in Bartlesville, OK (now called the National Institute for Petroleum and Energy Research (NIPER)) and at the Thermochemical Laboratory at Lund University, Lund, Sweden. The development of a high precision rotating bomb calorimeter was a key accomplishment which has led to the determination and publication of externely precise and accurate thermodynamic properties for CHS compounds. A rotating-bomb calorimeter is needed because the final state of sulfur as an aqueous sulfuric acid solution is not homogeneous in its dispersal throughout the interior of the static combustion bomb and is energetically uncertain. An important phase of the research effort focused on the establishment of the enthalpies of formation of aqueous sulfuric acid in various states of dilution. These $\Delta_t H^{\circ}$'s were then applied toward the identification of the final state of sulfur in the bomb combustion process for organic sulfur compounds. This feature is important because the energetics of the final thermodynamic state of the combustion process must be clearly and precisely defined. Without a knowledge of the final state of sulfur in the form of an aqueous sulfuric acid solution for the combustion reaction, highly precise and accurate data would not be available. For additional information, the reader should examine 56ROS, 62SKI, and 79SUN/ MAN.

The research effort in the two laboratories at Bartlesville and Lund was responsible for publication of high quality data available on organic sulfur compounds in the chemical literature and the subsequent good agreement found here between experimental and estimated values as presented in Tables 42 through 49.

Collectively, the residuals shown for thiols and sulfides are very small. Of the organic sulfur families, sulfones appear to be less well-behaved, but agreement here between experimental and estimated values is still reasonably good.

2.5. Organic Halogen Compounds

The families which comprise the CHX and CHXO compounds are: fluorides, chlorides, bromides, iodides, and mixed halogen compounds. A total of 258 halogen compounds are shown in Tables 50 through 54. Agreement between experimental and calculated values shows 54 percent of the residuals for $\Delta_t H^\circ$ to be $<\pm 4$ kJ·mol⁻¹, 17 percent to be $>\pm 4$ and $<\pm 8$ kJ·mol⁻¹, and 29 percent to be $>\pm 8$ kJ·mol⁻¹. For C_p° , 76 percent of the residuals are $<\pm 4$ J·mol⁻¹·K⁻¹, 11 percent are $>\pm 4$ but $<\pm 8$ kJ·mol⁻¹·K⁻¹, 17 percent are $>\pm 4$ but $<\pm 8$ J·mol⁻¹·K⁻¹, and 13 percent are $>\pm 4$ but $<\pm 8$ J·mol⁻¹·K⁻¹, and 13 percent are $>\pm 8$ J·mol⁻¹·K⁻¹.

In contrast to hydrocarbons and organic sulfur compounds, the thermodynamic properties of organic halogen compounds are collectively not known as precisely. In addition, halogen-halogen interactions operate which require interpetation. When these interactions are overlooked, they tend to make the differences between literature and estimated values larger than they should be.

The use of a rotating bomb calorimeter for the determination of enthalpies of combustion and for the derivation of enthalpies of formation is needed for organic halogen compounds. The enthalpy of formation of the final state of the hydrohalogen acid in aqueous solution must be determined in order to have a defined thermodynamic final state for the combustion process. Additional problems prevail with organic chlorine compounds in that they form about 15-20% elemental gaseous chlorine, Cl₂, and about 80-85% HCl in aqueous solution during the bomb combustion. A reducing agent such as a solution of arsenious oxide must be added to the combustion bomb prior to its closure with the sample so that the Cl₂ is converted to Cl⁻ and enters the aqueous solution. Similarly, without a reducing agent, organic bromine compounds form about 80-85% bromine, Br2, and 15-20% HBr in aqueous solution. Aqueous arsenious oxide reduces the Br₂ to aqueous HBr during the oxidation reaction when the reducing agent is added to the bomb prior to closure. The combustion process for organic fluorine compounds give aqueous HF as the only fluorine combustion product while organic iodine compounds yield crystalline elemental iodine as the singular iodine-containing product. For additional information, the reader should examine 56ROS, 62SKI, and 79SUN/MAN.

The large differences between the experimental and estimated values for $\Delta_t H^{\circ}(gas)$ and $\Delta_t H^{\circ}(solid)$ for decafluorobiphenyl (322.8 and 337.84 kJ·mol⁻¹, respectively) are not easily explained. The study reported by 79PRI/SAP2 for the combustion of $C_{12}F_{10}$ indicates that CO_2 , CF_4 , and F_2 are the only products of combustion in excess oxygen. Several reasons may explain the large differences. Possible explanations include: the energy corrections for the interactions between fluorine atoms in $C_{12}F_{10}$ may be different than those which are currently viewed; or, the quantitative determinations of the CF_4 and F_2 as combustion products may be in error.

We have attempted to correct for the interactions between halogen atoms in the various halogen families using cis-, ortho, or meta corrections, but success here is limited.

2.6. Comparison with an Extended Second-order Group Additivity Scheme

An extended multi-parameterized second-order group-additivity estimation scheme has been developed by J.B. Pedley and co-workers (86PED/NAY).

The Pedley scheme is limited to the estimation of enthalpies of formation of organic compounds at 298.15 K in the gas phase. The additional parameterization accounts more comprehensively for nearest- and next-to-nearest neighbor interactions than the estimation scheme developed by S.W. Benson and co-workers and used in this work.

The details of the Pedley scheme are discussed in a cursory manner in Appendix 3 and more fully in 86PED/NAY. A comparison of estimated values from the Pedley scheme and that used in this work has been made for 20 hydrocarbons and 20 organic oxygen compounds. The results indicate that differences between literature and estimated values are about the same for the two groups of compounds tested.

2.7. Summary and Conclusions

We have demonstrated the successful extension of the second-order group-additivity method for the estimation of $\Delta_t H^{\circ}$, C_p° , and S° at 298.15 K to liquid and solid organic compounds. A re-examination of group values for the gas phase was performed in order to maintain internal consistency with the condensed phase. This work has been carried out for 1512 organic compounds containing the elements carbon, hydrogen, oxygen, nitrogen, sulfur, and halogens. A total of over 3700 comparisons between literature and estimated values have been made for $\Delta_t H^\circ$, C_p° , and S° in the gas, liquid, and solid phases. Overall, for the compounds covered, the estimation of $\Delta_t H^{\circ}$ showed that 67 percent of the residuals were $< \pm 4 \text{ kJ} \cdot \text{mol}^{-1}$, 16 percent were $> \pm 4$ but $< \pm 8$ kJ·mol⁻¹, and 17 percent were $> \pm 8 \text{ kJ} \cdot \text{mol}^{-1}$. Values for C_p° showed that 80 percent of the residuals are < ±4 J·mol⁻¹·K⁻¹, 10 percent are $> \pm 4$ but $< \pm 8$ J·mol⁻¹·K⁻¹, and 10 percent are $> \pm 8 \text{ J·mol}^{-1} \cdot \text{K}^{-1}$. Values for S° show that 76 percent of the residuals are $< \pm 4$ J·mol⁻¹·K⁻¹, 14 percent are $> \pm 4$ but $<\pm 8$ J·mol⁻¹·K⁻¹, and 10 percent are $>\pm 8$ $J \cdot mol^{-1} \cdot K^{-1}$.

The groups and group values developed in this work should be helpful to thermochemists and chemical engineers for the estimation of enthalpies of formation, heat capacities, and entropies at 298.15 K and 101,325 Pa when their needs for predicted values of these thermodynamic properties arise. This estimation technique can also be used to establish whether a new experimentally determined value for $\Delta_t H^\circ$, C_p° , or S° comes within the range of expectations of group additivity as dictated by the experience already shown with this method.

Comparisons in Appendix 2 between literature values for the enthalpy and entropy of fusion and the enthalpy of vaporization, corrected from either T_m or T_b to 298.15 K, with corresponding differences $[\Delta_t H^{\circ}(\text{solid}) - \Delta_t H^{\circ}(\text{liq})]$, $[S^{\circ}(\text{solid}) - S^{\circ}(\text{liq})]$, and $[\Delta_t H^{\circ}(\text{liq}) - \Delta_t H^{\circ}(\text{g})]$, respectively, show that internal consistency does exist for the compounds tested.

The limited comparison of hydrocarbon and oxygencontaining compounds in Appendix 3 suggest that the extra effort taken in the Pedley scheme to account for nearest- and next-to-nearest neighbor interactions may have either a very small or even negligible effect upon reducing the degree of differences between literature and estimated values for enthalpies of formation at 298.15 K in the gas phase.

3. Tables of C-H-N-O-S-Halogen Compounds

TABLE 1. Summary of tables of C-H-N-O-S Halogen Families

Table 1.	C-H-N-O-S-Halogen Families	
Table 2.	Listing of Groups and Group Values	
Table 3.	General Definitions and Examples of Notations	
	for Molecular Groups	

Hydrocarbon Compounds

Table	Table Name Description		No. of Compounds
Table 4.	n- Alkanes	normal alkanes	25
Table 5.	t- alkanes	tertiary branched alkanes	35
Table 6.	q- Alkanes	quaternary branched alkanes	16
Table 7.	n-Alkenes	linear alkenes	32
Table 8.	s-Alkenes	branched alkenes	34
Table 9.	Alkynes	alkyne hydrocarbons	28
Table 10.	Aromatic CH-01	aromatic hydrocarbons	42
Table 11.	Aromatic CH-02	aromatic hydrocarbons	80
Table 12.	Cyclic CH-01	cyclic hydrocarbons	40
Table 13.	Cyclic CH-02	cyclic hydrocarbons	48
Table 14.	Cyclic CH-03	cyclic hydrocarbons	47
Total Hyd	rocarbon compounds		427

CHO Compounds

Table	Name	Description	No. of Compounds
Table 15.	Alcohols	alcohols, diols, triols, phenols	69
Table 16.	Ethers	linear, branched, and cyclic ethers	52
Table 17.	Aldehydes	aldehydes	16
Table 18.	Ketones	ketones	42
Table 19.	Acids	linear, branched, cyclic, and	
		aromatic acids	89
Table 20.	Anhydrides	anhydrides	11
Table 21.	Esters	esters and lactones	74
Table 22.	Peroxides	peroxides	7
Table 23.	Hydroperoxides	hydroperoxides	9
Table 24.	Peroxyacids	peroxyacids	8
Table 25.	Carbonates	carbonates	3
Total CH	O compounds		381

CHN Compounds

Table	able Name Description		No. of Compounds
Table 26.	Amines	Linear, branched, cyclic, aromatic	50
Table 27.	Imines	imines	2
Table 28.	Nitriles	linear, branched, cyclic, aromatic	27
Table 29.	Hydrazines	hydrazines	6
Table 30.	Diazenes	diazenes	14
Table 31.	Azides	azides	6
Table 32.	Cyclic CHN	heterocyclic nitrogen compounds	32
Total CH	N compounds		137

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TABLE 1. C-H-N-O-S-Halogen families (Continued)

CHNO Compounds

Table	Name	Description	No. of compound
Table 33.	Amides	Linear, Branched, Cyclic, Aromatic	28
Table 34.	Ureas	Ureas	24
Table 35.	Amino acids	Amino acids and peptides	38
Table 36.	Nitroso compounds	Nitroso and cyanato compounds	9
Table 37.	Nitro compounds	Linear, branched, cyclic, aromatic	50
Table 38.	Nitrites	Nitrites	3
Table 39.	Nitrates	Nitrates	6
Table 40.	Nitramines	Nitramines	10
Table 41.	Cyclic CHNO	Cyclic amides	3
Total CHI	NO compounds		171

CHS and CHSO Compounds

Table Name D		Description	No. of compounds
Table 42.	Thiols	Linear, branched, cyclic, aromatic	31
Table 43.	Sulfides	Linear, branched, aromatic	33
Table 44.	Disulfides	Disulfides	8
Table 45.	Sulfoxides	Sulfoxides	6
Table 46.	Sulfones	Linear, branched, aromatic	38
Table 47.	Sulfites	Sulfites	5
Table 48.	Sulfates	Sulfates	4
Table 49.	Cyclic CHS	Heterocyclic sulfur compounds	13
Total CHS a	and CHSO compounds		138

Halogen Compounds

Table	Name	Description	No. of compounds
Table 50.	Fluorides	CHF and CHFO compounds	46
Table 51.	Chlorides	CHCl and CHClO compounds	116
Table 52.	Bromides	CHBr and CHBrO compounds	39
Table 53.	Iodides	CHI and CHIO compounds	39
Table 54.	Mixed Halogen compounds	CHCIF, CHCIBr, CHBrF, CHFI compound	ls 18
Total Hale	ogen compounds		258
Total of a	ll compounds		1512

TABLE 2. Listing of groups and group values

Group	$\Delta_t H^\circ$ (gas)	C_p° (gas)	S° (gas)	$\Delta_{\mathrm{f}}H^{\circ}$ (liq)	C_p° (liq)	S° (liq)	$\Delta_t H^{\circ}$ (solid)	C_p° (solid)	S° (solid)
	(505)		CH Groups	(4)	(4)	(4)	(50114)	(30114)	(JOHU
C-(H) (C)	- 42.26	25.73	127.32	-47.61	36.48	83.30	- 46.74	67.45	56.69
C-(H) ₃ (C) C-(H) ₂ (C) ₂	- 42.20 - 20.63	22.89	39.16	-47.01 -25.73	30.48	32.38	- 40.74 - 29.41	21.92	23.01
C-(H)(C) ₃	-1.17	20.08	-53.60	-4.77	21.38	- 23.89	-5.98	-48.81	
-CH ₃ corr (tertiary)	-2.26	0.00	0.00	-2.18	0.00	0.00	-2.34	0.00	0.00
C-(C) ₄	19.20	16.53	- 149.49	17.99	10.24	-98.65	12.47	-83.63	
-CH ₃ corr (quaternary)	-4.56	0.00	0.00	- 4.39	0.00	0.00	-4.35	0.00	0.00
-CH ₃ corr (tert/quat)	-1.80	0.00	0.00	- 1.77	0.00	0.00	-2.70	0.00	0.00
-CH ₃ corr (quat/quat)	-0.64	0.00	0.00	-0.64	0.00	0.00	-2.24	0.00	0.00
C_{d} – $(H)_{2}$	26.32	21.38	115.52	21.75	28.37	86.19	22.43		
C _d -(H)(C)	36.32	18.74	33.05	31.05	24.60	28.58	25.48		
C _d -(C) ₂	44.14	15.10	-50.84	39.16	23.22	- 29.83	32.97		
C_{d} $(H)(C_{d})$	28.28	18.54	27.74	22.18	31.67	13.30	17.53	35.65	21.75
C_d – $(C)(C_d)$	36.78	17.57	-61.33	30.42	26.19	-41.92	27.91		
C_d - $(C_d)(C_B)$							56.07		
C_{d} -(H)(C_{B})	28.28	18.54	27.74	22.18	31.67	13.30	17.53	35.65	21.75
C_d -(C)(C_B)	37.95	15.90	- 51.97 27.74	38.58	21.67	12.20	17 52	25.65	21.75
C _d -(H)(C ₁) C-(H) ₄ , Methane	28.28 74.48	18.54 35.73	206.92	22.18	31.67	13.30	17.53	35.65	21.75
C_d – $(C_B)_2$	32.88	33.73	200.92	30.83	25.10		49.91	32.50	
$C-(H)_2(C)(C_d)$	-20.88	20.63	38.20	-25.73	29.29	31.67	-24.35	32.30	
$C-(H)(C)_2(C_d)$	-1.63	27.49	-50.38	-5.02	30.12	- 28.07	-6.49		
-CH ₃ corr (tertiary)	-2.26	0.00	0.00	-2.18	0.00	0.00	-2.34	0.00	0.00
C-(C) ₃ (C _d)	22.13	9.16	-150.23	20.79	28.74	-108.20	12.51	0.00	0.00
-CH ₃ corr (quaternary)	-4.56	0.00	0.00	- 4.39	0.00	0.00	-4.35	0.00	0.00
$C-(H)(C)(C_d)_2$	-1.17	20.08	- 53.60	-4.77	21.38	-23.89	-5.98	-48.81	- 16.89
$C-(H)_2(C_d)_2$	- 18.92	24.77	42.08	-24.43	40.88	19.32	-21.60		
$C-(H)_2(C_d)(C_B)$				-24.73					
$C-(H)(C)(C_d)(C_B)$	4.05	0.00		-6.90	0.00	0.00			
cis (unsat) corr	4.85	-8.03	5.06	5.27	0.00	0.00	5.73	0.00	0.00
tert-Butyl cis corr	17.24	0.00	0.00	17.48	0.00	0.00	17.57	0.00	0.00
C,-(H)	113.50	22.55	101.96	104.47	39.96	67.57	110.34		
C,-(C)	115.10	13.22	26.32	107.15	25.59	14.25	101.66		
C_t – (C_d)	121.42	10.71	39.92	114.77					
C_t - (C_B)	120.76	10.17	17.77	119.00			103.28	32.30	
G-(G)							103.28		
	120.76	14.27	25.94	104.80					
$C-(H)_2(C)(C_i)$	- 19.70	20.97	42.80	104.80 22.13	30.39	32.36	-29.41		
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁)	- 19.70 - 3.16	20.97 17.45	42.80 45.69	- 22.13				0.00	0.00
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary)	- 19.70	20.97	42.80	-22.13 -2.18	30.39 0.00	32.36 0.00	-2.34	0.00	0.00
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁)	-19.70 -3.16 -2.26	20.97 17.45 0.00	42.80 -45.69 0.00	-22.13 -2.18 22.83	0.00	0.00	-2.34 26.38		
$C-(H)_2(C)(C_1)$ $C-(H)(C)_2(C_1)$ $-CH_3$ corr (tertiary) $C-(C)_3(C_1)$ $-CH_3$ corr (quaternary)	- 19.70 - 3.16 - 2.26 - 4.56	20.97 17.45	42.80 45.69	-22.13 -2.18 22.83 -4.39			-2.34	0.00	0.00
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁)	-19.70 -3.16 -2.26	20.97 17.45 0.00	42.80 -45.69 0.00	-22.13 -2.18 22.83	0.00	0.00	-2.34 26.38		
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁) -CH ₃ corr (quaternary) C-(H) ₂ (C ₁) ₂ C-(C) ₂ (C ₁) ₂	- 19.70 - 3.16 - 2.26 - 4.56	20.97 17.45 0.00	42.80 -45.69 0.00	-22.13 -2.18 22.83 -4.39 -39.08 20.67	0.00	0.00	-2.34 26.38 -4.35		
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁) -CH ₃ corr (quaternary) C-(H) ₂ (C ₁) ₂ C-(C) ₂ (C ₁) ₂	- 19.70 - 3.16 - 2.26 - 4.56 - 41.14	20.97 17.45 0.00 0.00	42.80 - 45.69 0.00 0.00	-22.13 -2.18 22.83 -4.39 -39.08	0.00	0.00	-2.34 26.38		
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁) -CH ₃ corr (quaternary) C-(H) ₂ (C ₁) ₂ C-(C) ₂ (C ₁) ₂	- 19.70 - 3.16 - 2.26 - 4.56 - 41.14	20.97 17.45 0.00 0.00	42.80 - 45.69 0.00 0.00	- 22.13 - 2.18 22.83 - 4.39 - 39.08 20.67 134.68	0.00	0.00 0.00 14.39	-2.34 26.38 -4.35	0.00 20.13	0.00
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁) -CH ₃ corr (quaternary) C-(H) ₂ (C ₁) ₂ C-(C) ₂ (C ₁) C _n C _B -(H)(C _B) ₂	- 19.70 - 3.16 - 2.26 - 4.56 - 41.14 142.67 13.81	20.97 17.45 0.00 0.00	42.80 - 45.69 0.00 0.00 26.28 48.31	- 22.13 - 2.18 22.83 - 4.39 - 39.08 20.67 134.68 8.16	0.00 0.00 30.04 22.68	0.00 0.00 14.39 28.87	-2.34 26.38 -4.35	0.00 20.13	0.00 22.75 -5.50
C-(H ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁) -CH ₃ corr (quaternary) C-(H) ₂ (C ₁) ₂ C-(C) ₂ (C ₁) ₂ C C C C C C C C C C C C C C C C C C C	- 19.70 - 3.16 - 2.26 - 4.56 - 41.14 142.67 13.81 23.64 24.17 24.17	20.97 17.45 0.00 0.00 15.86 13.61 9.75 14.12	42.80 - 45.69 0.00 0.00 26.28 48.31 - 35.61 - 33.85 - 33.85	- 22.13 - 2.18 22.83 - 4.39 - 39.08 20.67 134.68 8.16 19.16 19.12 19.12	0.00 0.00 30.04 22.68 10.10 9.44 9.44	0.00 0.00 14.39 28.87 - 19.50	-2.34 26.38 -4.35 131.08 6.53 13.90 20.27 20.07	20.13 - 23.26 - 20.00 - 20.00	22.75 -5.50 -10.00
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁) -CH ₅ corr (quaternary) C-(H) ₂ (C ₁) ₂ C-(C) ₂ (C ₁) ₂ C _a C _b -(H)(C _b) ₂ C _b -(C)(C _b) ₂ C _b -(C ₁ (C _b) ₃	- 19.70 - 3.16 - 2.26 - 4.56 - 41.14 142.67 13.81 23.64 24.17	20.97 17.45 0.00 0.00 15.86 13.61 9.75 14.12	42.80 - 45.69 0.00 0.00 26.28 48.31 - 35.61 - 33.85	- 22.13 - 2.18 22.83 - 4.39 - 39.08 20.67 134.68 8.16 19.16 19.12	0.00 0.00 30.04 22.68 10.10 9.44	0.00 0.00 14.39 28.87 - 19.50 - 9.04	-2.34 26.38 -4.35 131.08 6.53 13.90 20.27 20.07 17.03	20.13 -23.26 -20.00	22.75 -5.50 -10.00
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁) -CH ₃ corr (quaternary) C-(H) ₂ (C ₁) ₂ C-(C) ₂ (C ₁) ₂ C _n C _B -(H)(C _B) ₂ C _B -(C)(C _B) ₂ C _B -(C ₁ (C ₀) ₂ C _C -(C ₁ (C ₀) ₂ C ₁ (C ₁ (C ₀) ₂ C ₁ (C ₁ (C ₀) ₂ C ₁ (C ₁ (C ₀) ₂ C ₂ (C ₁ (C ₀) ₂ C(C ₁ (C ₀) ₂ C(C ₁ (C ₀) ₂	- 19.70 - 3.16 - 2.26 - 4.56 - 41.14 142.67 13.81 23.64 24.17 24.17 21.66	20.97 17.45 0.00 0.00 15.86 13.61 9.75 14.12 13.12	42.80 - 45.69 0.00 0.00 26.28 48.31 - 35.61 - 33.85 - 36.57	- 22.13 - 2.18 22.83 - 4.39 - 39.08 20.67 134.68 8.16 19.16 19.12 19.12 17.21	0.00 0.00 30.04 22.68 10.10 9.44 9.44 17.07	0.00 0.00 14.39 28.87 -19.50 -9.04 -9.04	-2.34 26.38 -4.35 131.08 6.53 13.90 20.27 20.07 17.03 52.81	20.13 -23.26 -20.00 -20.00 -1.72	22.75 - 5.50 - 10.00 - 10.00 - 6.00
C-(H ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁) -CH ₃ corr (quaternary) C-(H) ₂ (C ₁) ₂ C-(C) ₂ (C ₁) ₂ C _n C _B -(H)(C _B) ₂ C _B -(C)(C _B) ₂ C _B -(C ₁ (C ₀) ₂ C _C -(C) ₂ (C ₀) ₂ C _C -(C) ₂ (C ₀) ₂ C _C -(C) ₂ (C ₀) ₂ C-(C) ₂ (C ₀) ₂ C-(H) ₂ (C)(C ₀)	- 19.70 - 3.16 - 2.26 - 4.56 - 41.14 142.67 13.81 23.64 24.17 24.17 21.66 - 21.34	20.97 17.45 0.00 0.00 15.86 13.61 9.75 14.12 13.12 25.61	42.80 -45.69 0.00 0.00 26.28 48.31 -35.61 -33.85 -36.57 42.59	- 22.13 - 2.18 22.83 - 4.39 - 39.08 20.67 134.68 8.16 19.16 19.12 19.12 17.21 - 24.81	0.00 0.00 30.04 22.68 10.10 9.44 17.07	0.00 0.00 14.39 28.87 -19.50 -9.04 -9.04	-2.34 26.38 -4.35 131.08 6.53 13.90 20.27 20.07 17.03 52.81 -22.10	20.13 - 23.26 - 20.00 - 20.00	22.75 -5.50 -10.00
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁) -CH ₃ corr (quaternary) C-(H) ₂ (C ₁) ₂ C-(C) ₂ (C ₁) ₂ C _n C _B -(H)(C _B) ₂ C _B -(C)(C _B) ₂ C _B -(C ₁ (C ₀) ₂ C _C -(C) ₂ (C _B) ₃ C-(C) ₂ (C _B) ₂	- 19.70 - 3.16 - 2.26 - 4.56 - 41.14 142.67 13.81 23.64 24.17 24.17 21.66	20.97 17.45 0.00 0.00 15.86 13.61 9.75 14.12 13.12	42.80 - 45.69 0.00 0.00 26.28 48.31 - 35.61 - 33.85 - 36.57	- 22.13 - 2.18 22.83 - 4.39 - 39.08 20.67 134.68 8.16 19.16 19.12 19.12 17.21	0.00 0.00 30.04 22.68 10.10 9.44 9.44 17.07	0.00 0.00 14.39 28.87 -19.50 -9.04 -9.04	-2.34 26.38 -4.35 131.08 6.53 13.90 20.27 20.07 17.03 52.81	20.13 -23.26 -20.00 -20.00 -1.72	22.75 - 5.50 - 10.00 - 10.00 - 6.00
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁) -CH ₃ corr (quaternary) C-(H) ₂ (C ₁) ₂ C-(C) ₂ (C ₁) ₂ C ₈ -(C) ₂ (C ₁) ₂ C ₈ -(C)(C ₈) ₂ C ₈ -(C)(C ₈) ₂ C ₈ -(C ₁ (C ₁) ₂ C ₈ -(C ₁ (C ₁) ₂ C ₈ -(C ₁ (C ₁) ₂ C ₁ -(C ₁ (C ₁) ₂ C ₁ -(C ₁ (C ₁) ₂ C ₂ -(C ₁ (C ₁) ₂ C ₃ -(C ₁ (C ₁) ₂ C ₄ -(C ₁ (C ₁) ₂ C ₆ -(C ₁ (C ₁) ₂ C ₇ -(H) ₂ (C)(C ₈) C-(H) ₂ (C)(C ₈) C-(H)(C) ₂ (C ₈) C-(C ₈ (C) ₃	- 19.70 - 3.16 - 2.26 - 4.56 - 41.14 142.67 13.81 23.64 24.17 21.66 - 21.34 - 4.52 18.28	20.97 17.45 0.00 0.00 15.86 13.61 9.75 14.12 14.12 13.12 25.61 22.45	42.80 -45.69 0.00 0.00 26.28 48.31 -35.61 -33.85 -36.57 42.59 -48.00	- 22.13 - 2.18 22.83 - 4.39 - 39.08 20.67 134.68 8.16 19.16 19.12 19.12 17.21 - 24.81 - 5.82 18.70	0.00 0.00 30.04 22.68 10.10 9.44 9.44 17.07 22.90 17.50 5.17	0.00 0.00 14.39 28.87 -19.50 -9.04 -9.04 47.40 -13.90 -96.10	-2.34 26.38 -4.35 131.08 6.53 13.90 20.27 20.07 17.03 52.81 -22.10 -3.50 21.57	20.13 -23.26 -20.00 -20.00 -1.72 49.38	22.75 -5.50 -10.00 -10.00 -6.00 26.90
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁) -CH ₃ corr (quaternary) C-(H) ₂ (C ₁) ₂ C-(C) ₂ (C ₁) ₂ C ₈ -(C) ₂ (C ₁) ₂ C ₈ -(C)(C ₈) ₂ C ₈ -(C)(C ₈) ₂ C ₈ -(C ₁ (C ₈) ₂ C ₈ -(C ₁ (C ₈) ₂ C ₈ -(C ₁ (C ₈) ₂ C ₁ (C ₁ (C ₈) ₂ C ₁ (C ₁ (C ₈) ₂ C ₁ (C ₁ (C ₈) ₂ C-(C) ₂ (C ₈) ₂ C-(H) ₂ (C(C ₈) ₂ C-(H) ₂ (C)(C ₈) C-(H)(C) ₂ (C ₈) C-(C ₁ (C ₁ (C ₈)	- 19.70 - 3.16 - 2.26 - 4.56 - 41.14 142.67 13.81 23.64 24.17 21.66 - 21.34 - 4.52	20.97 17.45 0.00 0.00 15.86 13.61 9.75 14.12 14.12 13.12 25.61 22.45	42.80 -45.69 0.00 0.00 26.28 48.31 -35.61 -33.85 -36.57 42.59 -48.00	- 22.13 - 2.18 22.83 - 4.39 - 39.08 20.67 134.68 8.16 19.16 19.12 19.12 17.21 - 24.81 - 5.82 18.70 - 26.50	0.00 0.00 30.04 22.68 10.10 9.44 9.44 17.07 22.90 17.50 5.17	0.00 0.00 14.39 28.87 -19.50 -9.04 47.40 -13.90 -96.10	-2.34 26.38 -4.35 131.08 6.53 13.90 20.27 20.07 17.03 52.81 -22.10 -3.50 21.57	20.13 - 23.26 - 20.00 - 20.00 - 1.72 49.38	22.75 - 5.50 - 10.00 - 10.00 - 6.00
C-(H) ₂ (C)(C ₁) C-(H)(C) ₂ (C ₁) -CH ₃ corr (tertiary) C-(C) ₃ (C ₁) -CH ₃ corr (quaternary) C-(H) ₂ (C ₁) ₂ C-(C) ₂ (C ₁) ₂ C _n C _n -(H)(C _n) ₂ C _n -(C)(C _n) ₂ C _n -(C) ₂ (C _n) ₂ C _n -(C) ₂ (C _n) ₂ C-(H) ₂ (C)(C _n) ₂ C-(H) ₂ (C)(C _n) ₂ C-(H)(C) ₂ (C _n) C-(H)(C) ₂ (C _n)	- 19.70 - 3.16 - 2.26 - 4.56 - 41.14 142.67 13.81 23.64 24.17 21.66 - 21.34 - 4.52 18.28	20.97 17.45 0.00 0.00 15.86 13.61 9.75 14.12 14.12 13.12 25.61 22.45	42.80 -45.69 0.00 0.00 26.28 48.31 -35.61 -33.85 -36.57 42.59 -48.00	- 22.13 - 2.18 22.83 - 4.39 - 39.08 20.67 134.68 8.16 19.16 19.12 19.12 17.21 - 24.81 - 5.82 18.70	0.00 0.00 30.04 22.68 10.10 9.44 9.44 17.07 22.90 17.50 5.17	0.00 0.00 14.39 28.87 -19.50 -9.04 -9.04 47.40 -13.90 -96.10	-2.34 26.38 -4.35 131.08 6.53 13.90 20.27 20.07 17.03 52.81 -22.10 -3.50 21.57	20.13 -23.26 -20.00 -20.00 -1.72 49.38	22.75 - 5.50 - 10.00 - 10.00 - 6.00 26.90

TABLE 2. Listing of groups and group values

		S° (gas)	Δ _t H° (lia)	Cp (lia)	S° (lia)	$\Delta_t H^\circ$ (solid)	C_p° (solid)	S° (solid)
(8-0)	(8)						(30114)	(5010
	0.00	0.00	15.02	0.50	5.54			
	0.00	0.00		9.52	-5.54			-6.00
								2.00
3.39			- 0.90				8.00	7.00
20.46								
22.46						47.93		
1.26	6.40	-2.50	3.26	3.50	0.00	5.00	0.00	0.00
-0.63	0.71	0.00	0.00	0.00	0.00	2.00	0.00	0.00
115 15	~ 12 73	134 86	111 58	- 28 53				
					51 /19	114.42		
						10.94		
	43.17	70.78		-27.00	2.90			
			41.33			46.27		
						.0.2,		
			24.83					
						37.48		
						65.09		
						67.14		
						69.56		
125.81	-11.67	126.77						
24.18	- 26.53	113.76	21.45	-15.82	48.37			
5.61	~ 19.50	95.69	2.04	-20.26	29.34			
21.81								
24.65			18.26					
				-26.56	50.18			
			3.04	34.22	50.41			
			36.42	-745	23 35			
	18.63	102.26						
248.50	- 19.97	286.59	242.58	2.60	162.81			
105.05								
	07.07	110.00		00.00				
						10.30		
								0.00
								0.00
0.00	16.48	-23.00	0.00	0.00	0.00	0.00	0.00	0.00
127.00	- 183.44		-4.02	-54.12	53.75			
123.81	-183.24		-15.22	-57.63	53.67			
19.51			16.39					
				. 3.00		55.06	- 24 02	
99.35						109.46	- 24.92 - 4.02	
125.09						177 26	_ 12 19	_ 1 02
125.09 50.95						127.26 65.53		-1.92
125.09 50.95 6.14						127.26 65.53 3.18	- 13.18 14.90	-1.92
	-0.63 115.15 110.89 26.75 0.68 26.34 40.65 52.91 51.99 47.56 17.31 21.84 49.37 8.03 8.41 -13.59 223.26 125.81 24.18 5.61 21.81 24.65 24.07 17.14 -2.69 27.54 39.34 16.84 71.37 248.50 105.95 19.55 -0.39 24.31 0.00 0.00 0.00 127.00 123.81 19.51 15.16 52.08	27.04 20.10 16.00 3.59 22.46 1.26 -0.63 0.71 115.15 -12.73 110.89 -19.34 26.75 -31.44 0.68 -31.07 26.34 -37.14 40.65 -43.17 52.91 51.99 47.56 17.31 21.84 49.37 8.03 8.41 -13.59 223.26 125.81 -11.67 24.18 -26.53 5.61 -19.50 21.81 24.65 24.07 17.14 -2.69 27.54 39.34 16.84 -18.63 71.37 -26.31 248.50 -19.97 105.95 19.55 -27.87 -0.39 -22.82 24.31 -24.50 0.00 11.83 0.00 14.39 0.00 16.48 127.00 -183.44 123.81 -183.24 19.51 15.16 52.08	(gas) (gas) (gas) CH Groups 27.04 20.10 0.00 0.00 16.00 3.59 22.46 1.26 6.40 -2.50 -0.63 0.71 0.00 115.15 -12.73 134.86 110.89 -19.34 126.04 26.75 -31.44 116.22 0.68 -31.07 78.18 26.34 -37.14 73.97 40.65 -43.17 70.78 52.91 51.99 47.56 17.31 21.84 49.37 8.03 8.41 -13.59 223.26 125.81 -11.67 126.77 24.18 -26.53 113.76 5.61 -19.50 95.69 21.81 24.65 24.07 17.14 -2.69 27.54 39.34 16.84 -18.63 102.26 71.37 -26.31 116.38 248.50 -19.97 286.59 105.95 19.55 -27.87 118.39 -0.39 -22.82 83.97 24.31 -24.50 117.11 0.00 11.83 -19.66 0.00 14.39 -21.50 0.00 16.48 -23.00 127.00 -183.44 123.81 -183.24 19.51 15.16 52.08	CH Groups CH Groups 27.04 20.10 0.00 15.83 16.00 3.59 -0.90 22.46 1.26 6.40 -2.50 3.26 -0.63 0.71 0.00 0.00 115.15 -12.73 134.86 111.58 110.89 -19.34 126.04 106.64 26.75 -31.44 116.22 22.84 0.68 -31.07 78.18 -1.77 26.34 -37.14 73.97 23.50 40.65 -43.17 70.78 38.10 52.91 50.61 47.55 17.31 21.84 24.83 49.37 8.03 8.41 -13.59 223.26 125.81 -11.67 126.77 24.18 -26.53 113.76 21.45 5.61 -19.50 95.69 2.04 21.81 24.65 18.26 24.07 23.95 17.14	CH Groups	CH Groups CH Groups 27.04 20.10 0.00 0.00 15.83 9.52 -5.54 16.00 11.50 3.59 -0.90 -0.90 22.46 1.26 6.40 -2.50 3.26 3.50 0.00 -0.63 0.71 0.00 0.00 0.00 0.00 0.00 115.15 -12.73 134.86 111.58 -28.53 1110.89 -19.34 126.04 106.64 -10.68 51.48 26.75 -31.44 116.22 22.84 -23.32 42.24 0.68 -31.07 78.18 -1.77 -26.21 10.07 26.34 -37.14 73.97 23.50 -32.19 15.89 40.65 -43.17 70.78 38.10 -27.88 2.96 52.91 50.61 47.55 17.731 21.84 24.83 49.37 8.38 1.93 49.37 8.38 1.93 48.37 5.61 -15.82 48.37 5.61 -15.82<	CH Groups CH Groups 27.04 20.10 0.00 15.83 9.52 -5.54 44.89 20.10 0.00 0.00 11.583 9.52 -5.54 14.10 16.00 3.59 -0.90 1.20 -8.77 -8.77 -8.77 22.46 -2.50 3.26 3.50 0.00 5.00 -8.77 1.26 6.40 -2.50 3.26 3.50 0.00 5.00 -0.63 0.71 0.00 0.00 0.00 0.00 2.00 115.15 -12.73 134.86 111.58 -28.53 114.41 14.43 26.75 -31.44 116.02 22.84 -23.32 42.24 34.00 0.68 -31.07 78.18 -1.77 -26.21 10.07 10.94 26.34 -37.14 73.97 23.50 -32.19 15.89 40.65 -43.17 70.78 <td>CH Groups CH Groups</td>	CH Groups CH Groups

TABLE 2. Listing of groups and group values - Continued

Group	$\Delta_t H^{\circ}$ (gas)	C_p° (gas)	S° (gas)	$\Delta_t H^\circ$ (liq)	C_p° (liq)	S° (lig)	$\Delta_t H^{\circ}$ (solid)	C_p° (solid)	S° (solid)
	-		CH Groups				·		
Bicyclo[2,2,2]octane rsc	27.12				-67.59	-63.45	41.52		
Bicyclo[3.3.3]undecane rsc	99.06						124.10		
cis-Bicyclo[6.1.0]nonane rsc	115.55			109.35					
Bicyclo[1.1.0]butane rsc	260.70			254.70					
Bicyclo[3.1.0]hexane rsc	123.16			117.56					
Bicyclo[2.2.1]hepta-2,5-diene rsc	125.29			124.87					
Tetracyclo-[3.2.02,7.04,6]heptane rsc	366.75			356.45					
Tricyclo[2.2.1.02,6]heptane rsc	148.67			139.67					
Bicyclo[2.2.1]hept-2-ene rsc	82.79			73.58			102.73		
Bicyclo[2.2.1]heptane rsc	43.49			45.39			57.01		
Bicyclo[4.1.0]heptane rsc	106.99			101.39					
Pentacyclo-[4.2.0.02,5.03,8.04,7]-octane rsc	674.60						632.84		
Bicyclo[2.2.2]oct-2-ene rsc	33.64						56.36		
Bicyclo[4.2.0]octane rsc	100.72			95.72					
Bicyclo[5.1.0]octane rsc	109.42			103.62					
trans-Bicyclo[6.1.0]nonane rsc	107.05			107.25					
Bicyclo[3.3.1]nonane rsc	19.25			27.02			39.63		
cis-Bicyclo[3.3.0]octane rsc	33.22 59.52			27.92 54.72					
trans-Bicyclo[3.3.0]octane rsc	J9.J2								
		c	HO Group	s					
CO-(H) ₂ , Formaldehyde	- 108.60	35.40	224.54		<u></u>		······································		************
CO-(C)(CO)	- 121.29			- 135.04			- 140.75		
CO-(H)(CO)	- 105.98								
$CO-(CO)(C_B)$	-112.30						- 117.75		
CO-(O)(CO)	-123.75			-123.30	40.63		-120.81		
$CO-(C^q)(O)$	- 136.73	24.56	62.59	- 155.56	48.16		- 134.10	43.75	32.90
CO-(C)(O)	-137.24	24.56	62.59	- 149.37	44.98	32.72	- 153.60	44.98	32.13
CO-(H)(O)	- 124.39	29.00	147.03	-142.42	65.10	94.68	400.00		
CO-(O) ₂	-111.88			-122.00	31.46		- 123.00	4.25	- 42.92
CO – $(H)(C_d)$ CO – $(C_B)_2$	126.96 110.00			153.05 119.00			- 116.00	109.33	
CO-(C)(C _B)	- 148.82			-145.22	73.35		- 143.70	71.38	23.72
CO-(H)(C _B)	- 121.35			-138.12	54.22		- 160.18	40.55	
$CO-(O)(C_B)$	- 125.00			- 140.00	48.16		- 145.00	43.75	32.13
CO-(C) ₂	-132.67	23.43	64.31	-152.76	52.97	33.81	- 157.95		
CO-(H)(C)	-124.39	29.00	147.03	-142.42	65.10	93.55			
CO-(C)(C _d)					27.07				
O-(CO) ₂ , aliphatic	-214.50	-1.08	34.16	-230.50	5.28		-235.00		
O-(CO) ₂ , aromatic	-238.30			-220.90			-207.00		
O-(C _d)(CO)	- 198.03			-201.42	19.58				
0-(C)(C0)	- 188.87	11.80	36.03	-196.02	19.58	38.28	-210.60	-6.00	12.09
O-(H)(CO) O-(C _B)(CO)	- 254.30 - 167.00	16.23	101.71	-285.64 -165.50	37.82	38.28	- 282.15 - 170.00	44.60 29.08	21.78 45.32
0-(C)(O)	- 107.00 - 20.75			- 103.50 - 23.50			- 170.00 - 30.20	29.00	43.32
O-(H)(O)	- 72.26			- 101.75			- 105.30		
$O-(C_d)_2$	- 139.29			-137.32			102.20		
O-(H)(C _d)					37.78				
O-(C)(C _d)	- 129.33			-133.72	51.21				
O-(C _B) ₂	-77.66			-85.27		23.31	- 96.20	15.90	3.14
$O-(C)(C_B)$	-92.55			-104.85	8.10		-122.87		
$O-(H)(C_B)$	-160.30	18.16	121.50	- 191.75	44.64	43.89	- 199.25	29.25	28.62
O-(C) ₂	-101.42	18.54	29.33	-110.83	24.27	26.78	-119.00		
O-(H)(C)	- 159.33	18.16	121.50	-191.50	44.64	43.89	- 199.66	29.25	28.62
C _d -(H)(CO) C _d -(C)(CO)	32.30	15.61	35.19	26.61	28.12 18.62		7.82	- 18.66	27.53

TABLE 2. Listing of groups and group values - Continued

Group	Δ _t H° (gas)	C_p° (gas)	S° (gas)	$\Delta_t H^\circ$ (liq)	C_p° (liq)	S° (liq)	$\Delta_t H^{\circ}$ (solid)	C_{ρ}° (solid)	S° (solid)
			CHO Group						-
C (0)(C)	36.78	17.57	-61.34	30.42	26.19	-41.92	27.91		
C_d – $(O)(C_d)$ C_d – $(O)(C)$	30.76 44.14	17.37	- 50.84	39.08	23.22	-41.92 -29.83	32.97		
C ₄ -(O)(H)	36.32	18.74	33.05	31.05	24.60	28.58	25.48		
G (GO)							144.50		
C_1 -(CO) C_B -(CO)(C_B) ₂	15.50			10.50	4.39		144.52 8.15	- 42.89	0.08
C_B (CO)(C_B) ₂	-4.75	15.86	-43.72	-5.61	39.71	- 10.59	1.00	-0.29	1.59
C (II) (CO)	20.74			22.06	15 56		10.10		
C-(H) ₂ (CO) ₂ C-(CO)(C) ₃	-30.74 23.93			-23.06 26.15	15.56 7.99	85.98	- 19.10 24.02	- 114.10	
C-(H)(CO)(C) ₂	-0.25			- 3.89	17.41	- 24.52	- 9.83	- 80.51	
C-(H) ₂ (CO)(C)	-21.84	24.69	39.58	- 24.14	29.29	39.87	- 27.90	21.92	24.73
C-(H) ₃ (CO)	- 42.26	25.73	127.32	- 47.61	36.48	83.30	- 46.74	67.45	56.69
C-(H) ₂ (CO)(C _d)	- 16.95	23.13	127.52	- 19.62	30.40	05.50	40.74	07.43	30.03
C-(H) ₂ (CO)(C ₁)	-25.48			-26.61					
C-(H) ₂ (CO)(C _B)	-16.20			- 11.67					
$C-(H)(CO)(C)(C_B)$	10.20			11.07			14.81		
C-(H)(O)(CO)(C)	126.63			123.43	7.44	-46.71	- 14.39	- 58.45	8.08
C-(O)4	- 152.46			-133.34		10.72	14.05	30.43	0.00
C-(H)(O) ₃	- 113.97			-107.74	21.71				
C-(O) ₃ (C)	- 114.39			99.54					
$C-(O)_2(C)_2$	-53.56			-41.30					
$C-(H)(O)_2(C)$	-57.78			-51.42	12.38				
$C-(H)_2(O)_2$	-62.22			-62.89	39.92	23.85			
$C-(H)_2(O)(C_B)$	-33.76			-29.17	46.48				
$C-(H)_2(O)(C_d)$	-27.49	17.74	37.49	-28.62	41.30				
$C-(H)(CO)(C)(C_B)$							-14.39		
$C-(H)(CO)(C_B)_2$							3.72		
$C-(O)(C_B)_3$							60.46	57.49	
C-(O)(C) ₃ (ethers, esters)	9.50	14.60	- 141.92	0.79	20.46	- 94.68	-0.50		
C-(H)(O)(C) ₂ (ethers, esters)	- 19.46	17.78	-52.80	-21.00	25.56	-25.31	-20.08		
C-(O)(C) ₃ (alcohols, peroxides)	- 13.50	15.73	- 144.60	-11.13	65.58	-122.48	-12.25	-85.48	- 14.77
C-(H)(O)(C) ₂ (alcohols, peroxides)	-26.10	19.96	-43.05	-27.60	49.83	- 29.83	-29.08	4.77	6.95
C-(H) ₂ (O)(C)	-32.90	20.33	43.43	-35.80	33.64	32.59	-33.00	21.92	24.73
C-(H) ₃ (O)	-42.26	25.73	127.32	- 47.61	36.48	83.30	- 46.74	67.45	56.69
O-(CO)(O)	-88.00			-90.00			-80.50		
$C-(C)_2(O)(C_B)$	15.30			25.80			29.30		
$C-(H)(C)(O)_2$							-52.50		
Glutaric anhydride rsc	20.89						8.91		
Succinic anhydride rsc	4.76			-11.08			-10.60		
Phthalic anhydride rsc	30.66						-5.52		
Cyclopentanone rsc	22.85			15.10					
Cyclohexanone rsc	10.50	-31.82	66.98	5.60	-25.61	11.29			
Cycloheptanone rsc	10.76			6.31					
Cyclooctanone rsc	7.33			9.01			37.38		
Cyclononanone rsc	20.43			22.57			55.28		
Cyclodecanone rsc	15.70			17.73					
Cycloundecanone rsc	19.39			20.53					
Cyclododecanone rsc	12.91			18.02			47.11		
Cyclopentadecanone rsc Cycloheptadecanone rsc	9.41 4.87						74.77 89.49		
Cyclobutane-1,3-dione rsc									
Ethylene oxide rsc	140.48 114.62	~ 10.02	122 00	104 92	_ 22 00	00 E0	94.10		
Trimethylene oxide rsc	114.62 107.35	- 10.92	132.00	104.82	-23.90	80.50			
Furan rsc	- 12.18			- 9.97	-22.38				
Tetrahydrofuran rsc	24.28	-28.73	113.66	- 9.97 17.70	- 28.49	47.18	14.60		
Tetrahydropyran rsc	5.71	20.13	113.00			77.10			
1 cuanyuropyran rsc	5./1			1.32	-42.22		0.80		

TABLE 2. Listing of groups and group values - Continued

Group	$\Delta_t H^\circ$ (gas)	C_p° (gas)	S° (gas)	$\Delta_t H^\circ$ (liq)	<i>C</i> ° (liq)	S° (liq)	$\Delta_t H^\circ$ (solid)	C_{ρ}° (solid)	S° (solid
		C	CHO Groups	<u></u>					
1,3-Dioxolane rsc	29.06			18.75	-37.74				
1,3-Dioxane rsc	10.90			4.40	-42.26				
1,4-Dioxane rsc	19.15	- 24.34	73.16	9.76	-29.50	86.28	- 12.00		
1,3-Dioxepane rsc	25.52			20.01	- 49.20				
Trioxane rsc	25.02								
Tetraoxane rsc	34.23								
β-Propiolactone rsc	97.95			75.43	-5.40	31.85			
τ-Butyrolactone rsc	34.98			10.16	- 16.61	21.56			
τ-Valerolactone rsc δ-Valerolactone rsc	26.06 42.51			4.75 19.19	- 16.74	10.77			
o-valerolactone isc	42.31			19.19	- 10.74	10.77			
Caprolactone rsc					-21.92	-4.92			
Undecanolactone rsc Ethylene carbonate rsc					-28.12	-33.05	23.90		
Cyclobutane methyl carboxylate rsc	75.21			79.08			23.90		
Bicyclobutane methyl carboxylate rsc	73.21 222.27			219.98					
Dicyclobutane methyr carooxylate 150	<i>666.61</i>			217.70					
1,4-Dimethylcubane dicarboxylate rsc	595.80						590.73		
2-Deoxy-D-ribose rsc							0.25		
β-D-Ribose rsc							12.65		
α-D-Glucose rsc							6.30		
COOH-COOH (ortho corr)							34.14	15.00	8.96
COOH-COOH (meta corr)	-23.94						13.14	30.00	0.00
CH ₃ O-COOH (ortho corr)	15.00						23.00		
CH ₃ O-COOH (meta corr) OH-OH (ortho corr)	5.00 7.00						5.00 16.00		
OH-OH (meta corr)	0.00						2.00		
OH-COOH (ortho corr)	-20.00						0.00		
		CHN a	nd CHNO	jroups					
C-(H) ₃ (N)	- 42.26	25.73	127.32	-47.61	36.48	83.30	-46.74	67.45	56.69
C-(H) ₂ (C)(N)	-28.30	22.68	42.26	- 30.80	30.42	32.38	-34.00	21.92	23.01
C-(H)(C) ₂ (N)	- 16.70	18.62 0.00	- 63.55	- 14.65	28.28 0.00	- 20.00 0.00	- 13.90 - 2.34	0.00	0.00
-CH ₃ corr (tertiary) C-(C) ₃ (N)	-2.26	0.00			LILES	U.UU			11(0)
			0.00 152 59	-2.18 5.10				0.00	0.00
-U.H. corr (quaternary)	0.29 4.56	18.41	- 152.59	5.10	19.66	-87.99	1.00	-84.14	
-CH ₃ corr (quaternary) C-(H) ₂ (N) ₂	-4.56						1.00 4.35		0.00
-CH ₃ corr (quaternary) C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N)		18.41	- 152.59	5.10	19.66	-87.99	1.00	-84.14	
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N)	-4.56 -30.00 -24.14	18.41 0.00	- 152.59 0.00	5.10 -4.39 -26.09	19.66 0.00 19.79	- 87,99 0.00	1.00 -4.35 -26.00 -33.31	- 84.14 0.00	0.00
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids)	-4.56 -30.00 -24.14	18.41 0.00 24.35	- 152.59 0.00	5.10 -4.39 -26.09	19.66 0.00 19.79 62.59	-87.99 0.00 71.71	1.00 -4.35 -26.00 -33.31	-84.14 0.00	0.00 39.00
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids) N-(H) ₂ (C) (second, amino acids)	-4.56 -30.00 -24.14 19.25 19.25	18.41 0.00	- 152.59 0.00	5.10 -4.39 -26.09	19.66 0.00 19.79	- 87,99 0.00	1.00 -4.35 -26.00 -33.31	- 84.14 0.00	0.00
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids)	-4.56 -30.00 -24.14	18.41 0.00 24.35 24.35	- 152.59 0.00 124.40 126.90	5.10 -4.39 -26.09 0.33 0.33	19.66 0.00 19.79 62.59 62.59	-87.99 0.00 71.71 71.71	1.00 -4.35 -26.00 -33.31 -6.30 -46.00	-84.14 0.00 32.00 71.27	0.00 39.00
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids) N-(H) ₂ (C) (second, amino acids) N-(H)(C) ₂ N-(C) ₃	-4.56 -30.00 -24.14 19.25 19.25 67.55 116.50	18.41 0.00 24.35 24.35 12.28 15.10	- 152.59 0.00 124.40 126.90 33.96 - 61.71	5.10 -4.39 -26.09 0.33 0.33 51.50 112.00	19.66 0.00 19.79 62.59 62.59 59.37 26.11	-87.99 0.00 71.71 71.71 32.09 -38.62	1.00 -4.35 -26.00 -33.31 -6.30 -46.00 47.80 101.00	-84.14 0.00 32.00 71.27 -8.00	0.00 39.00
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids) N-(H) ₂ (C) (second, amino acids) N-(H)(C) ₂ N-(C) ₃ N-(H) ₂ (N)	-4.56 -30.00 -24.14 19.25 19.25 67.55 116.50	18.41 0.00 24.35 24.35 12.28	- 152.59 0.00 124.40 126.90 33.96	5.10 -4.39 -26.09 0.33 0.33 51.50	19.66 0.00 19.79 62.59 62.59 59.37	-87.99 0.00 71.71 71.71 32.09	1.00 -4.35 -26.00 -33.31 -6.30 -46.00 47.80	-84.14 0.00 32.00 71.27 -8.00	0.00 39.00
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids) N-(H) ₂ (C) (second, amino acids) N-(H)(C) ₂ N-(C) ₃ N-(H) ₂ (N) N-(H)(C)(N)	-4.56 -30.00 -24.14 19.25 19.25 67.55 116.50	18.41 0.00 24.35 24.35 12.28 15.10	- 152.59 0.00 124.40 126.90 33.96 - 61.71	5.10 -4.39 -26.09 0.33 0.33 51.50 112.00 25.30	19.66 0.00 19.79 62.59 62.59 59.37 26.11	-87.99 0.00 71.71 71.71 32.09 -38.62 60.58	1.00 -4.35 -26.00 -33.31 -6.30 -46.00 47.80 101.00	-84.14 0.00 32.00 71.27 -8.00	0.00 39.00
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids) N-(H) ₂ (C) (second, amino acids) N-(H)(C) ₂ N-(C) ₃ N-(H) ₂ (N)	-4.56 -30.00 -24.14 19.25 19.25 67.55 116.50 47.70 89.16	18.41 0.00 24.35 24.35 12.28 15.10	- 152.59 0.00 124.40 126.90 33.96 - 61.71	5.10 -4.39 -26.09 0.33 0.33 51.50 112.00 25.30 75.00	19.66 0.00 19.79 62.59 62.59 59.37 26.11 49.41 49.04	71.71 71.71 32.09 -38.62 60.58 22.05	1.00 -4.35 -26.00 -33.31 -6.30 -46.00 47.80 101.00	-84.14 0.00 32.00 71.27 -8.00	0.00 39.00
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids) N-(H) ₂ (C) (second, amino acids) N-(H)(C) ₂ N-(C) ₃ N-(H) ₂ (N) N-(H)(C)(N) N-(C) ₂ (N) N-(C _B) ₂ (N) N-(C _B) ₂ (N) N-(H)(C _B)(N)	-4.56 -30.00 -24.14 19.25 19.25 67.55 116.50 47.70 89.16	18.41 0.00 24.35 24.35 12.28 15.10	- 152.59 0.00 124.40 126.90 33.96 - 61.71	5.10 -4.39 -26.09 0.33 0.33 51.50 112.00 25.30 75.00	19.66 0.00 19.79 62.59 62.59 59.37 26.11 49.41 49.04	71.71 71.71 32.09 -38.62 60.58 22.05	1.00 -4.35 -26.00 -33.31 -6.30 -46.00 47.80 101.00 18.97	-84.14 0.00 32.00 71.27 -8.00	0.00 39.00
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids) N-(H) ₂ (C) (second, amino acids) N-(H)(C) ₂ N-(C) ₃ N-(H) ₂ (N) N-(H)(C)(N) N-(C) ₂ (N) N-(C) ₃ (N)	-4.56 -30.00 -24.14 19.25 19.25 67.55 116.50 47.70 89.16 120.71	18.41 0.00 24.35 24.35 12.28 15.10	- 152.59 0.00 124.40 126.90 33.96 - 61.71	5.10 -4.39 -26.09 0.33 0.33 51.50 112.00 25.30 75.00 119.00	19.66 0.00 19.79 62.59 62.59 59.37 26.11 49.41 49.04	71.71 71.71 32.09 -38.62 60.58 22.05	1.00 -4.35 -26.00 -33.31 -6.30 -46.00 47.80 101.00 18.97	-84.14 0.00 32.00 71.27 -8.00	0.00 39.00
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids) N-(H) ₂ (C) (second, amino acids) N-(H)(C) ₂ N-(C) ₃ N-(H) ₂ (N) N-(H)(C)(N) N-(C) ₂ (N) N-(C _B) ₂ (N) N-(H)(C _B)(N) N-(H)(C _B)(N) N-(H)(C _B)(N)	-4.56 -30.00 -24.14 19.25 19.25 67.55 116.50 47.70 89.16 120.71	18.41 0.00 24.35 24.35 12.28 15.10	- 152.59 0.00 124.40 126.90 33.96 - 61.71	5.10 -4.39 -26.09 0.33 0.33 51.50 112.00 25.30 75.00 119.00	19.66 0.00 19.79 62.59 62.59 59.37 26.11 49.41 49.04	71.71 71.71 32.09 -38.62 60.58 22.05	1.00 -4.35 -26.00 -33.31 -6.30 -46.00 47.80 101.00 18.97	-84.14 0.00 32.00 71.27 -8.00	0.00 39.00
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids) N-(H) ₂ (C) (second, amino acids) N-(H)(C) ₂ N-(C) ₃ N-(H) ₂ (N) N-(H)(C)(N) N-(C) ₂ (N) N-(C _B) ₂ (N) N-(C _B) ₂ (N) N-(H)(C _B)(N)	-4.56 -30.00 -24.14 19.25 19.25 67.55 116.50 47.70 89.16 120.71 87.50	18.41 0.00 24.35 24.35 12.28 15.10	- 152.59 0.00 124.40 126.90 33.96 - 61.71	5.10 -4.39 -26.09 0.33 0.33 51.50 112.00 25.30 75.00 119.00 73.40	19.66 0.00 19.79 62.59 62.59 59.37 26.11 49.41 49.04	71.71 71.71 32.09 -38.62 60.58 22.05	1.00 -4.35 -26.00 -33.31 -6.30 -46.00 47.80 101.00 18.97	-84.14 0.00 32.00 71.27 -8.00	0.00 39.00
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids) N-(H) ₂ (C) (second, amino acids) N-(H)(C) ₂ N-(C) ₃ N-(H) ₂ (N) N-(H)(C)(N) N-(C) ₂ (N) N-(C _B) ₂ (N) N-(H)(C _B)(N) N-(CO) ₂ (N) N-(H)(C _d) ₂ N-(C)(C _d) ₂	-4.56 -30.00 -24.14 19.25 19.25 67.55 116.50 47.70 89.16 120.71 87.50 83.55 120.64	18.41 0.00 24.35 24.35 12.28 15.10 26.36	- 152.59 0.00 124.40 126.90 33.96 - 61.71 122.18	5.10 -4.39 -26.09 0.33 0.33 51.50 112.00 25.30 75.00 119.00 73.40	19.66 0.00 19.79 62.59 62.59 59.37 26.11 49.41 49.04 41.67	-87.99 0.00 71.71 71.71 32.09 -38.62 60.58 22.05 -26.94	1.00 -4.35 -26.00 -33.31 -6.30 -46.00 47.80 101.00 18.97 137.35 66.90 73.62 45.40 88.92	-84.14 0.00 32.00 71.27 -8.00 -39.00	0.00 39.00 48.75
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids) N-(H) ₂ (C) (second, amino acids) N-(H)(C) ₂ N-(C) ₃ N-(H) ₂ (N) N-(H)(C)(N) N-(C) ₂ (N) N-(C _B) ₂ (N) N-(C _B) ₂ (N) N-(CO) ₂ (N) N-(H)(C _d) ₂ N-(C)(C _d) ₂ N-(H) ₂ (C _B)	-4.56 -30.00 -24.14 19.25 19.25 67.55 116.50 47.70 89.16 120.71 87.50 83.55 120.64	18.41 0.00 24.35 24.35 12.28 15.10	- 152.59 0.00 124.40 126.90 33.96 - 61.71	5.10 -4.39 -26.09 0.33 0.33 51.50 112.00 25.30 75.00 119.00 73.40 50.50 97.38 -11.00	19.66 0.00 19.79 62.59 62.59 59.37 26.11 49.41 49.04 41.67	71.71 71.71 32.09 -38.62 60.58 22.05	1.00 -4.35 -26.00 -33.31 -6.30 -46.00 47.80 101.00 18.97 137.35 66.90 73.62 45.40 88.92 -21.60	-84.14 0.00 32.00 71.27 -8.00 -39.00	0.00 39.00
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids) N-(H) ₂ (C) (second, amino acids) N-(H)(C) ₂ N-(C) ₃ N-(H) ₂ (N) N-(H)(C)(N) N-(C) ₂ (N) N-(C _B) ₂ (N) N-(C _B) ₂ (N) N-(CO) ₂ (N) N-(H)(C _d) ₂ N-(C)(C _d) ₂ N-(H) ₂ (C _B) N-(H)(C(C _B)	-4.56 -30.00 -24.14 19.25 19.25 67.55 116.50 47.70 89.16 120.71 87.50 83.55 120.64 19.25 59.00	18.41 0.00 24.35 24.35 12.28 15.10 26.36	- 152.59 0.00 124.40 126.90 33.96 - 61.71 122.18	5.10 -4.39 -26.09 0.33 0.33 51.50 112.00 25.30 75.00 119.00 73.40 50.50 97.38 -11.00 26.25	19.66 0.00 19.79 62.59 62.59 59.37 26.11 49.41 49.04 41.67	-87.99 0.00 71.71 71.71 32.09 -38.62 60.58 22.05 -26.94	1.00 -4.35 -26.00 -33.31 -6.30 -46.00 47.80 101.00 18.97 137.35 66.90 73.62 45.40 88.92 -21.60 36.55	-84.14 0.00 32.00 71.27 -8.00 -39.00	0.00 39.00 48.75
C-(H) ₂ (N) ₂ C-(H) ₂ (C _B)(N) N-(H) ₂ (C) (first, amino acids) N-(H) ₂ (C) (second, amino acids) N-(H)(C) ₂ N-(C) ₃ N-(H) ₂ (N) N-(H)(C)(N) N-(C) ₂ (N) N-(C _B) ₂ (N) N-(C _B) ₂ (N) N-(CO) ₂ (N) N-(H)(C _d) ₂ N-(C)(C _d) ₂ N-(H) ₂ (C _B)	-4.56 -30.00 -24.14 19.25 19.25 67.55 116.50 47.70 89.16 120.71 87.50 83.55 120.64	18.41 0.00 24.35 24.35 12.28 15.10 26.36	- 152.59 0.00 124.40 126.90 33.96 - 61.71 122.18	5.10 -4.39 -26.09 0.33 0.33 51.50 112.00 25.30 75.00 119.00 73.40 50.50 97.38 -11.00	19.66 0.00 19.79 62.59 62.59 59.37 26.11 49.41 49.04 41.67	-87.99 0.00 71.71 71.71 32.09 -38.62 60.58 22.05 -26.94	1.00 -4.35 -26.00 -33.31 -6.30 -46.00 47.80 101.00 18.97 137.35 66.90 73.62 45.40 88.92 -21.60	-84.14 0.00 32.00 71.27 -8.00 -39.00	0.00 39.00 48.75

TABLE 2. Listing of groups and group values - Continued

Group	Δ _f H°	C _p °	S°	Δ _t H°	C _p °	S°	Δ _t H°	C _p °	S°
•	(gas)	(gas)	(gas)	(liq)	(liq)	(liq)	(solid)	(solid)	(solid)
		CHN a	and CHNO	Groups			· · · · · · · · · · · · · · · · · · ·		
N-(C _B) ₃	123.15			121.80			107.50	- 39.00	
N _r -(C)	81.46			73.68					
$N_{\Gamma}(C_B)$	69.00	10.07	47.01	54.50	19.75	36.40	57.00		
N _A -(C)	109.50			104.85			103.00		
N _A -(C _B)	109.50			104.85			103.00		
N _A -(oxide)(C)	40.80			22.65					
$C-(H)_2(C)(N_A)$	-20.70			-25.70			-29.41		
$C-(H)(C)_2(N_A)$	-2.66			-5.42					
$C-(C)_3(N_A)$	11.50			15.50			10.50		
C _d -(H)(N)	- 16.00			- 15.50			- 13.00		
C_{d} –(C)(N)	-5.74			-5.62			-3.95		
$C_B-(N)(C_B)_2$	-1.30	16.07	-43.53	1.50	15.02	-24.43	9.75	13.00	- 37.57
C_B -(NO)(C_B) ₂	21.50						23.00		
C_B -(NO_2)(C_B) ₂	-1.45			- 28.30	73.30	79.95	-32.50	50.96	110.46
C_B -(CNO)(C_B) ₂	- 177.63						155.69		
$C_B-(CN)(C_B)_2$	151.00	41.09	85.25	122.38	51.80	64.75	121.20		50.45
C_B - $(N_A)(C_B)_2$	22.55			20.08			18.65		
$C_B-(H)(N_I)_2$	6.30						0.25		
CO-(H)(N)	- 124.39	29.00	147.03	-188.00	65.10	93.55			
CO-(C)(N)	- 133.26	22.50	56.70	-185.00	49.16		194.60	39.00	40.00
CO-(C _B)(N) (amides)							- 177.75	111.50	
CO-(C _B)(N) (amino acids)	- 171.80						- 177.75	37.00	
$CO-(C_d)(N)$ $CO-(N)_2$	-171.80 -111.00	32.40	96.00	- 190.50			-203.10	124.00	69.00
(11)2	111.00	32.40	70.00	170.50			- 205.10	124.00	05.00
N-(H) ₂ (CO) (amides, ureas)	-63.00	17.00	88.25	-63.90	43.01		-65.25	- 15.50	18.00
N-(H) ₂ (CO) (amino acids)	-63.00			-63.90	43.01		59.75	45.88	33.03
N-(H)(C)(CO) (amides, ureas)	- 16.28			-17.10	23.51		-9.80	-36.00	
N-(H)(C)(CO) (amino acids)	- 16.28 45.00			- 17.10 62.00	23.51 13.93		5.50	3.30	
N-(C) ₂ (CO) N-(H)(C _B)(CO)	- 20.84			62.00	13.93		55.00 -3.50	-41.00	
	20.04						-3.30	-41.00	
N-(H)(CO) ₂	-91.00			***			- 30.80	- 157.02	
N-(C)(CO) ₂	-11.64			56.20			64.00		
N-(C _B)(CO) ₂	9.12						(0.05		
$N-(C_B)_2(CO)$ $N-(C)(C_B)(CO)$							60.85		
C-(H) ₃ (CN), Acetonitrile	74.04	52.22	252.60	40.56	91.46	149.62	72.00		
C-(H) ₂ (C)(CN)	94.52	47.86	167.25	66.07	83.01	106.02	69.85	72.80	96.15
C-(H)(C) ₂ (CN)	113.50	44.94	67.86	81.50	83.09	200.02	69.00	72.00	70.15
C-(C) ₃ (CN)	137.96			116.20	69.91	-17.91	102.07		
$C-(C)_2(CN)_2$								44.60	74.57
$C-(H)_2(C_d)(CN)$	95.31			66.40					
C_d -(H)(CN)	146.65	42.38	158.41	117.28	80.42	92.72			
C,-(CN)	264.60			250.20					
C-(H) ₃ (NO ₂), Nitromethane	- 74.86	57.32	284.14	-112.60	105.98	171.75			
C-(H) ₂ (NO ₂) ₂ , Dinitromethane	-58.90			-104.90					
C-(H)(NO ₂) ₃ , Trinitromethane	-0.30			-32.80			48.00		
C-(NO ₂) ₄ , Tetranitromethane	82.30			38.30					
$C-(H)_2(C)(NO_2)$	- 60.50	53.14	203.60	-93.50	97.74		- 99.00		
$C-(H)(C)_2(NO_2)$	- 53.00	49.58	115.32	-82.50			-89.00		
C-(C) ₃ (NO ₂)	- 36.65			-61.20			- 76.55		
$C-(H)_2(C_B)(NO_2)$	- 62.00			-82.76			-81.00		
C-(H)(C)(NO ₂) ₂	- 36.80			- 88.80			-91.50		
C-(C) ₂ (NO ₂) ₂	- 28.50			-77.20			- 90.30	71.38	,
C-(H)(C)(CO)(N)	- 18.70 - 3.10						-11.65	-22.85	-4.00
C-(H) ₂ (CO)(N)	-3.10						- 30.95	21.92	24.00
$C-(H)(C_B)(CO)(N)$								61.21	

TABLE 2. Listing of groups and group values - Continued

Group	$\Delta_t H^\circ$ (gas)	C_p° (gas)	S° (gas)	$\Delta_{\mathrm{f}}H^{\circ}$ (liq)	C_p° (liq)	S° (liq)	$\Delta_{f}H^{\circ}$ (solid)	C_p° (solid)	S° (solid
	(gas)				(114)	(nq)	(sonu)	(Soliu)	(801)
		CHN a	nd CHNO	Groups					
O-(C)(NO)	- 24.23	37.49	166.11	-46.50	06.40	107.50	124.00		
O-(C)(NO ₂)	<i> 79.7</i> 1	51.46	191.92	- 108.96	96.40	127.50	- 124.00		
N-(H)(C)(NO ₂) N-(H)(C _B)(NO ₂)							-16.50	65.73 -47.53	
N-(H)(CO)(NO ₂)							- 14.00		
$N-(C)(NO_2)_2$	100.30			53.50			4 = 0 = 0		
$N-(C)(C_B)(NO_2)$ $N-(C)_2(NO)$	183.00 90.00			167.00 59.00			150.50 55.00		
N-(C) ₂ (NO ₂)	88.00			50.00			40.00		
C-(H) ₂ (C)(N ₃)				321.70					
$C-(H)(C)_2(N_3)$	274.00			255.00					
$C-(H)_2(C_B)(N_3)$	347.00			327.40					
$C-(C_B)_3(N_3)$	328.60						346.50		
C_{B} - $(N_3)(C_B)_2$	320.00			303.50					
Zwitterion energy, aliphatic	0.00	0.00	0.00	0.00	0.00	0.00	-55.10	- 44.50	
Zwitterion energy, aromatic I	0.00	0.00	0.00	0.00	0.00	0.00	- 32.00	-20.50	
Zwitterion energy, aromatic II Ethyleneimine rsc	0.00	0.00	0.00	0.00	0.00	0.00	-11.00	5.00	-9.00
Pyrrolidine rsc	115.53 26.71	-5.13 -22.29	137.90 118.45	101.98 20.36	-24.48	42.40			
Piperidine rsc	3.14	- 22.23	110.43	- 1.09	- 24.46 - 29.79	15.98			
Hexamethyleneimine rsc	3.14			1.07	-36.86	13.70			
Octahydroazocine rsc					-42.31				
Pyrrolizidine rsc	35.42			18.87					
3,5-Dimethylpyrrolizidine rsc	38.46			20.05					
Trimethyl cyanurate rsc	- 95.00						- 120.40		
Succinimide rsc	25.70						16.70		
Glutarimide rsc	28.23						17.57		
Azetidine rsc	116.00			102.00					
Pyrrole rsc	- 30.48			-20.03			-17.84		
Cyclotetramethylenediazene rsc Cyclotrimethylenediazene rsc	12.86 - 10.47			-4.34			- 23.97		
•							23.77		
Cyclopropanenitrile rsc	110.56			110.76	-28.53				
Cyclobutanenitrile rsc	91.39			98.69	-28.35				
Cyclopentanenitrile rsc Cyclohexanenitrile rsc	10.82 -5.55			22.12 -0.05	- 37.27 - 57.29				
Cyclonexamemitine 1sc	-3.33			-0.03	-31.29				
N-Nitrosopiperidine rsc	45.20			48.70					
N-Nitropiperidine rsc	- 13.91			-4.11			8.48		
R-salt rsc RDX rsc	32.00						195.30 30.00		
HMX rsc	32.00 17.00						32.00		
DINO-PMTA rsc	17.00						46.70		
cis-Azobenzene corr	48.40						49.10		
Azidocyclopentane rsc	29.42			27.02					
Azidocyclohexane rsc	-16.45			-17.95					
NO ₂ -NO ₂ (ortho corr)	44.00			45.25			40.60	3.76	
NO ₂ -NO ₂ (meta corr)	11.00			13.50			13.50	5.84	
NO ₂ -CH ₃ (ortho corr)	2.00			2.00			4.00		
NO ₂ -CH ₃ (meta corr)				-4.00					
NO ₂ -OH (ortho corr)	10.00			16.00			13.00		
NO ₂ -OH (<i>meta</i> corr) NO ₂ -NO ₂ (aliphatic-adjacent corr)	6.00			20.00			0.00 20.00		
	20.00 25.00			20.00 30.00			25.00	0.00	
NO ₂ -COOH (ortho corr)									

TABLE 2. Listing of groups and group values - Continued

Group	$\Delta_{\rm f}H^{\circ}$ (gas)	C_p° (gas)	S° (gas)	Δ _t H° (lig)	C_{ρ}° (liq)	S° (liq)	$\Delta_{i}H^{\circ}$ (solid)	C_p° (solid)	S° (solid
	(600)		and CHNO		(4)	()	(sona)	(30114)	(SONG
NO OW days	10.00			·			12.00		
NO ₂ -OH(ortho corr)	10.00 6.00			16.00 0.00			13.00		
NO ₂ -OH(meta corr) NH ₂ -NO ₂ (ortho corr)	-4.00			-4.00			0.00 4.00	0.00	
NH ₂ -NO ₂ (orno corr) NH ₂ -NO ₂ (meta corr)	-10.00			-10.00			- 4.00 - 10.00	0.00	
(ONO ₂)-(ONO ₂)(aliphatic-adjacent corr)	15.10			15.90			16.00		
N _I -(CH ₃) (ortho corr)	-6.30			-4.00					
N _I -N _I (ortho corr)	85.06			83.16					
CH₃-CN (cis, unsat corr)	-6.00			~6.00					
NH ₂ -NH ₂ (ortho corr)							-3.00		
NH ₂ -NH ₂ (meta corr)				10.00			- 10.00		
NH ₂ -COOH (ortho corr)				12.00			14.00	-4.71	
NH ₂ -COOH (meta corr)				2.00			4.00	-7.22	
		CHS a	nd CHSO	Groups					
C-(H) ₃ (S)	-42.26	25.73	127.32	-47.61	36.48	83.30	-46.74	67.45	56.69
C-(H) ₂ (C)(S)	-23.17	20.90	41.87	- 26.77	24.18	41.09			
C-(H)(C) ₂ (S)	-5.88	20.29	-47.36	-6.07	17.78	-16.61			
-CH ₃ corr (tertiary)	-2.26	0.00	0.00	-2.18	0.00	0.00	-2.34	0.00	0.00
C-(C) ₃ (S)	13.52 - 4.56	17.02 0.00	- 145.38 0.00	16.69 4.39	8.88	-86.86	4.25	0.00	0.00
-CH ₃ corr (quaternary) -CH ₃ corr (tert/quat)	- 4.30 - 1.80	0.00	0.00	-4.39 -1.77	0.00 0.00	0.00 0.00	-4.35 -2.70	0.00	0.00
-CH ₃ corr (quat/quat)	- 1.60 - 0.64	0.00	0.00	-0.64	0.00	0.00	- 2.70 - 2.24	0.00 0.00	0.00
C-(H) ₂ (C _B)(S)	- 18.53	0.00	0.00	-23.82	0.00	0.00	- 2.24	0.00	0.00
C-(H) ₂ (C _d)(S)	- 25.93			- 32.44					
C-(H) ₂ (S) ₂	-25.10								
C_B – $(S)(C_B)_2$	-4.75	15.86	43.72	-5.61	39.71	- 10.59	1.00	-0.29	1.59
C_{d} -(H)(S)	36.32	18.74	33.05	31.05	24.60	28.58	25.48		2.07
C _d -(C)(S)	45.73	14.64	-51.92						
S-(C)(H)	18.64	25.76	137.67	0.06	51.34	85.95			
S-(C _B)(H)	48.10	20.98	57.34	28.51	20.11	89.04			
S-(C) ₂	46.99	22.64	55.19	29.82	45.15	29.80			
$S-(H)(C_d)$	25.52								
$S-(C)(C_d)$	54.39								
S-(C _d) ₂	102.60	20.04	68.59						
S-(C _B)(C)	76.21	02.05	50.50	58.20	16.43	35.44	42.00		
S-(C)(S)	27.62	23.25	50.50	14.36	40.71	30.84			
$S-(C_B)(S)$	57.45						40.60		
S-(S) ₂	12.59	19.66	56.07						
$S-(C_B)_2$	102.60	20.04	68.59	93.02	-35.10				
S-(H)(S) S-(H)(CO)	7.95 5.90	31.92	130.54						
				150.76	50.00	22.01			
CO-(C)(S)	- 132.67	23.43	64.31	-152.76	52.97	33.81		33.89	
C−(H)₃(SO) C−(H)₂(C)(SO)	- 42.26 - 29.16	25.73	127.32	- 47.61 - 36.88	36.48	83.30	-46.74	67.45	56.69
C-(H)(C) ₂ (SO)	.10			20.00					
-CH ₃ corr (tertiary)	-2.26	0.00	0.00	-2.18	0.00	0.00	-2.34	0.00	0.00
C-(C) ₃ (SO)	4.56	5.00	3.00	0.97	5.00	3.00	≥. ∓	0.00	0.00
-CH ₃ corr (quaternary)	-4.56	0.00	0.00	-4.39	0.00	0.00	-4.35	0.00	0.00
$C-(H)_2(C_d)(SO)$	-27.56			- 32.63					
cis correction	4.11	-8.03	5.06	5.27	0.00	0.00	5.73	0.00	0.00
C_B –(SO)(C_B) ₂	15.48			25.44	4.39		7.55	- 42.89	0.08
O-(SO)(H)	- 158.60								

TABLE 2. Listing of groups and group values - Continued

Group	Δ _f H°	C _p	S°	$\Delta_t H^\circ$	C _p °	S°	Δ _f H°	C _p °	S°
	(gas)	(gas)	(gas)	(liq)	(liq)	(liq)	(solid)	(solid)	(solid
		CHS a	nd CHSO	Groups					
SO-(C) ₂	- 66.78	37.15	75.73	-108.98	80.22	22.18			
SO-(C _B) ₂	- 62.26								
SO-(O) ₂	-213.00								
SO-(C)(C _B)	- 72.00								
C-(H) ₃ (SO ₂)	-42.26	25.73	127.32	- 47.61	36.48	83.30	- 46.74	67.45	56.69
$C-(H)_2(C)(SO_2)$	-27.03			-33.76		,	- 35.96		
$C-(H)(C)_2(SO_2)$	- 14.00								
-CH ₃ corr (tertiary)	-2.26	0.00	0.00	- 2.18	0.00	0.00	-2.34	0.00	0.00
C-(C) ₃ (SO ₂)	1.52			2.00			3.78		
-CH ₃ corr (quaternary)	-4.56	0.00	0.00	-4.39	0.00	0.00	-4.35	0.00	0.00
-CH ₃ corr (quat/quat)	-0.64			- 0.64			-2.24		
$C-(H)_2(C_d)(SO_2)$	- 29.49			-49.05					
$C-(H)(C)(C_d)(SO_2)$	-71.99								
$C-(H)_2(C_B)(SO_2)$	-29.80								
C-(H) ₂ (C ₁)(SO ₂)	16.36			25.44	4.20		255	40.00	0.00
C_B -(SO ₂)(C_B) ₂ C_d -(H)(SO ₂)	15.48 51.58			25.44	4.39		7.55	-42.89	0.08
C_d -(H)(SO ₂) C_d -(C)(SO ₂)	64.01								
C ₁ -(SO ₂)	177.10								
SO_2 -(C_d)(C_B)	-291.55								
SO ₂ -(C _d)(C _B)	-306.70								
SO ₂ -(C _d) ₂ SO ₂ -(C) ₂	-288.58	48.54	87.37	-341.14			- 356.62	- 9.55	32.10
SO ₂ -(C)(C _B)	- 289.10	10.5 1	0,157	01111			330.02	7.55	32.10
SO ₂ -(C _B) ₂	-287.76						- 305.40		
SO_2 - $(SO_2)(C_B)$	-325.18						- 361.75		
SO ₂ -(O) ₂	-417.30								
SO_2 -(C)(C _d)	-316.80								
SO_2 -(C_t)(C_B)	- 296.30								
O-(SO ₂)(H)	-158.60								
O-(C)(SO ₂)	- 91.40								
Thiacyclopropane rsc	81.57	- 10.76	122.10	75.32					
Thiacyclobutane rsc	80.98	- 18.00	112.89	74.55	-10.54	40.57			
Thiacyclopentane rsc	6.41	- 19.34	97.87	2.08	-14.19	31.08			
Thiacyclohexane rsc	-2.02	-24.91	66.85	~ 5.09	-21.47	9.12			
Thiacycloheptane rsc	20.53	-31.40	66.35	13.84					
2,5-Dihydrothiophene rsc Thiophene rsc	19.13 43.54	-1.59	22.79	19.96					
2,3-Dihydrothiophene rsc	7.72	-1.59	. 24.13						
		CHX a	nd CHXO	Groups					
C_(H) (F) Mathyl flygrids	- 247.00		231.93						
C-(H) ₃ (F), Methyl fluoride C-(H) ₃ (Cl), Methyl chloride	- 247.00 - 81.90	37.49 40.75	231.93						
C-(H) ₃ (CI), Methyl chloride C-(H) ₃ (Br), Methyl bromide	- 81.90 - 37.66	40.75 42.43	243.60 254.94	-61.10					
C-(H) ₃ (I), Methyl iodide	14.30	44.14	263.14	-11.70	82.76				
C-(C)(F) ₃	- 673.81	52.99	178.22	- 709.07	73.18	135.56			
C-(H) ₂ (C)(F)	- 221.12	33.66	146.80						
$C-(H)_2(C)(F)$ $C-(H)(C)_2(F)$	- 221.12 - 204.46	30.55	55.76						
C-(C) ₃ (F)	- 202.92	50.55	33.70						
C-(H)(C)(F) ₂	- 454.74	42.22	164.32	-487.23	68.04				
C-(C) ₂ (F) ₂	- 411.39	41.42	74.48	-400.37	00.07		- 428.77		
C-(C)(Cl)(F) ₂	- 462.70	57.32	169.45	-466.00	83.64	138.31			
C-(H)(C)(Cl)(F)	-271.14								
C-(C)(Cl) ₃	-81.98	68.18	202.14	-112.93	102.20	145.91			
C-(H)(C)(Cl) ₂	-79.10	50.69	183.28	-102.60	85.02	128.45			

TABLE 2. Listing of groups and group values - Continued

Group	$\Delta_t H^\circ$ (gas)	C° (gas)	S° (gas)	$\Delta_{\mathfrak{t}}H^{\circ}$ (liq)	C° (liq)	S° (liq)	$\Delta_t H^\circ$ (solid)	Cp° (solid)	S° (solid)
	(6)		and CHXO		(4)	. (4)	(33.12)	(00.12)	(50110)
G (T) (O)(O)	CO.15			· · · · · · · · · · · · · · · · · · ·		404.05	0.5.4.5		
$C-(H)_2(C)(Cl)$ $C-(C)_2(Cl)_2$	- 69.45 - 79.56	37.53 54.40	159.24 95.41	- 86.90 - 101.80	63.76 74.24	104.27	-85.65		
$C-(C)_2(CI)_2$ $C-(H)(C)_2(CI)$	- 55.61	35.00	71.34	- 71.17	66.02				
C-(C) ₃ (Cl)	- 43.70	29.63	-24.26	- 56.78	00.02				
C-(C)(Br) ₃		69.87	233.05						
$C-(H)(C)(Br)_2$									
$C-(H)_2(C)(Br)$	-21.78	37.82	173.31	-42.65	66.00	113.00			
$C-(C)_2(Br)_2$									
$C-(H)(C)_2(Br)$	- 10.75	36.77	84.69	- 27.31	59.24				
C-(C) ₃ (Br)	7.26	39.33	- 13.46	-7.40					
C-(C)(I) ₃	400 00	54.04	222.45						
$C-(H)(C)(I)_2$	108.78	51.04	228.45		(5.0)				
$C-(H)_2(C)(I)$	33.54	40.94	177.78	4.14	65.36		3.65		
$C-(C)_2(I)_2$ $C-(H)(C)_2(I)$	48.74	38.62	88.10	24.78					
$C-(II)(C)_2(I)$ $C-(C)_3(I)$	68.46	41.09	- 3.21	48.60					
C (C)3(1)	00.40	11.07	5.21	10.00					
-C-(H)(C)(Br)(Cl)	- 18.45 - 32.64	51.88	191.21						
$N-(C)(F)_2$ C-(H)(C)(CI)(O)	- 32.04 - 90.37	37.66	66.53						
C-(H) ₂ (I)(O)	15.90	37.00	170.29						
C-(C)(Cl) ₂ (F)	- 322.54		2,0.25	-343.87	89.29	141.71			
C-(C)(P-)(E)	- 394.55				85.40	140.70			
$C-(C)(Br)(F)_2$ $C-(C)(Br)_2(F)$	- 394.33				85.40	149.70			
C-(Br)(Cl)(F)									
C_{d} -(H)(F)	- 165.12	28.45	137.24						
C _d -(H)(Cl)	4.37	32.75	147.85	- 12.67	56.62				
C_{d} -(H)(Br)	50.94	34.10	159.91		79.13				
C_{d} -(H)(I)	102.36	36.82	169.45						
C_d –(C)(Cl)	-5.06		62.76	- 2.23					
C_d - $(F)_2$	- 329.90	39.43	155.63						
C _d -(Cl) ₂	- 11.51	46.86	175.41	-32.08	76.47	115.35			
C_d – $(Br)_2$ C_d – $(I)_2$		51.46	199.16						
C_d -(Cl)(F)	- 235.10	44.50	175.61						
C (P-)(P)		45.40	155.00						
C_d -(Br)(F)		45.19	177.82						
C _d -(Cl)(Br) C _t -(F)	•	50.63	188.70						
C ₁ -(Cl)		33.01	140.00						
C_t -(Br)		34.69	151.30						
C ₁ -(I)	35.53	158.41							
C_B - $(F)(C_B)_2$	- 181.26	26.10	67.52	- 191.20	37.09	54.19	- 194.00	32.05	39.79
C_B -(Cl)(C_B) ₂	- 17.03	29.33	77.08	-32.20	35.27	55.47	-32.00	33.55	43.37
C_B -(Br)(C_B) ₂	36.35	29.65	88.60	19.90	40.91	74.85	13.50		54.45
$C_B-(I)(C_B)_2$	94.50	32.70	98.26	73.70	45.17	61.08	70.40	40.08	
cis corr-(I)(I)	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C-(H) ₂ (CO)(CI)	-44.26			- 58.41			- 74.75		
C-(H)(CO)(Cl) ₂	- 40.40			-55.11					
CO-(C)(F)	- 379.84	50.00	150.00	-419.59					
$C-(C_B)(F)_3$ $C-(H)_2(C_B)(Br)$	691.79 29.49	52.30	179.08	696.66 44.06					
$C-(H)_2(C_B)(I)$ $C-(H)_2(C_B)(I)$	7.31			- 44.06 - 7.24					
$C-(H)_2(C_B)(C_I)$	-73.79			- 92.56					
CO-(C)(Cl)	- 200.54	42.09	176.66	- 225.29	80.67				
$CO-(C_B)(Cl)$	20001		5.55	-216.67	69.21		-212.99		
CO_(C)(P+)	140 54			176 40					
CO-(C)(Br)	148.54 83.94			-175.49					
CO-(C)(I)	- 83.94			- 117.09					

TABLE 2. Listing of groups and group values - Continued

Group	$\Delta_{\mathrm{f}}H^{\circ}$	C _p °	S°	$\Delta_t H^\circ$	C_p°	S°	$\Delta_t H^\circ$	C _p °	S°
• •	(gas)	(gas)	(gas)	(liq)	(liq)	(liq)	(solid)	(solid)	(solid
		CHX ar	d CHXO	Groups					
C-(H)(C)(CO)(Cl)	-39.88			-35.46	49.45				
$C-(C)(CO)(CI)_2$					74.22				
ortho corr-(I)(I)	7.56	0.00	0.00	6.96	0.00	0.00	5.50	0.00	0.00
ortho corr-(F)(F)	20.90	0.00	0.00	25.00	0.00	0.00	25.50	0.00	0.00
ortho corr-(Cl)(Cl)	9.50	0.00	0.00	14.00	0.00	0.00	8.50	0.00	0.00
ortho corr-(alkyl)(X)	2.51	0.00	0.00	6.30	0.00	0.00	0.00	0.00	0.00
cis corr-(Cl)(Cl)	-4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
cis corr-(CH ₃)(Br)	-4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ortho corr-(F)(Cl)	13.50	0.00	0.00	18.50	0.00	0.00	19.50	0.00	0.00
ortho corr-(F)(Br)	37.25	0.00	0.00	40.60	0.00	0.00	42.50	0.00	0.00
ortho corr-(F)(I)	85.40	0.00	0.00	83.55	0.00	0.00	85.20	0.00	0.00
meta corr-(I)(I)	0.00	0.00	0.00	0.00	0.00	0.00	20.08	0.00	0.00
meta corr-(COCl)(COCl)	0.00	0.00	0.00	0.00	0.00	0.00	16.06	0.00	0.00
ortho corr-(COCl)(COCl)	0.00	0.00	0.00	0.00	10.58	0.00		0.00	0.00
ortho corr-(F)(CF ₃)	111.00	0.00	0.00	112.00	0.00	0.00	0.00	0.00	0.00
meta corr-(F)(CF ₃)	2.00	0.00	0.00	6.00	0.00	0.00	0.00	0.00	0.00
ortho corr-(F)(CH ₃)	-3.30	0.00	0.00	-6.00	0.00	0.00	0.00	0.00	0.00
ortho corr-(F)(F')	8.00	0.00	0.00	8.00	0.00	0.00	8.00	0.00	0.00
ortho corr-(Cl)(Cl')	8.00	0.00	0.00	8.00	0.00	0.00	8.00	0.00	0.00
meta corr-(F)(F)	0.00	0.00	0.00	6.00	0.00	0.00	8.50	0.00	0.00
meta corr-(Cl)(Cl)	-5.00	0.00	0.00	10.00	0.00	0.00	4.00	0.00	0.00
ortho corr-(Cl)(CHO)	-6.75	0.00	0.00	8.50	0.00	0.00	0.00	0.00	0.00
ortho corr-(F)(COOH)	20.00	0.00	0.00	0.00	0.00	0.00	20.00	0.00	0.00
ortho corr-(Cl)(COCl)	0.00	0.00	0.00	34.43	0.00	0.00	0.00	0.00	0.00
ortho corr-(F)(OH)	25.50	0.00	0.00	23.00	0.00	0.00	20.00	0.00	0.00
ortho corr-(Cl)(COOH)	0.00	0.00	0.00	0.00	0.00	0.00	20.00	0.00	0.00
ortho corr-(Br)(COOH)	0.00	0.00	0.00	0.00	0.00	0.00	20.00	0.00	0.00
ortho corr-(I)(COOH)	0.00	0.00	0.00	0.00	0.00	0.00	20.00	0.00	0.00
ortho corr-(NH ₂)(NH ₂)	- 10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
meta corr-(NH ₂)(NH ₂)	0.00	0.00	0.00	0.00	0.00	0.00	14.00	0.00	0.00
ortho corr-(OH)(Cl)	7.50	0.00	0.00	0.00	0.00	0.00	11.00	0.00	0.00
cis corr-(CH ₃)(I)	-4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Group identities

```
C-(H)_3(C)
C-(H)(C_3)
                        = C-(H)(C)(C_d)_2
                         = C_{d^{-}}(H)(O) = C_{d^{-}}(H)(S) 
 = C_{d^{-}}(H)(C_{t}) = C_{d^{-}}(H)(C_{B}) = C_{d^{-}}(O)(C_{d}) 
C_{\sigma}-(H)
C_d-(H)(C<sub>d</sub>)
                        C_B-(H)(C_B)_2
                        = C_{B^{-}}(C)(S)(C_{B})
C_B-(C_d)(C_B)<sub>2</sub>
                        = C_{B} - (C_t)(C_B)_2
C_B-(SO)(C_B)<sub>2</sub>
                        = C_B - (SO_2)(C_B)_2
S-(C_d)_2
                        = S-(C_B)_2
```

TABLE 3. General definitions and examples of notations for organic groups

C-(H) ₃ (C)	A carbon atom with three bonds to hydrogen atoms and the fourth bond to a carbon atom. Example: Ethane.
$C-(H)_2(C)_2$	A carbon atom with two bonds to hydrogen atoms and two bonds to carbon atoms. Example: n-Hexane.
C-(H)(C) ₃	A carbon atom with one bond to a hydrogen atom and three bonds to carbon atoms. Example: 2-Methylpropane.
C-(C) ₄	A carbon atom with four bonds to carbon atoms. Example: 2,2-Dimethylpropane.
C _d -(H) ₂	A doubly-bonded carbon atom attached to two hydrogen atoms. Example: Ethylene.
C _d -(C) ₂	A doubly-bonded carbon atom attached to two carbon atoms. Example: Propene.
C _i -(H)	A triply-bonded carbon atom attached to a hydrogen atom. Example: Ethyne.
C ₁ -(C)	A triply-bonded carbon atom attached to a carbon atom. Example: Propyne.
C_B -(H)(C_B) ₂	An aromatic ring (benzene) carbon atom bonded to a hydrogen atom and two other aromatic ring carbon atoms. Example: Benzene.
C_B – $(C_B)_3$	An aromatic ring (benzene) carbon atom bonded to three aromatic ring carbon atoms. Example: Biphenyl.
C_{BF} $(C_{BF})(C_B)_2$	A fused aromatic ring carbon atom (such as the two fused ring carbon atoms in naphthalene) bonded to one other fused aromatic ring carbon atom and aromatic ring carbon atoms. Example: Naphthalene.
C_{BF} – $(C_{BF})_3$	A fused aromatic ring carbon atom bonded to three other fused aromatic ring carbon atoms. Example: Pyrene.
C_a	An allenic carbon atom. When allene is unsubstituted, the group values are equal to allene itself. Example: Allene.
-CH ₃ corr (tertiary)	A correction for the attachment of each methyl group to a tertiary carbon atom. Example: 2-Methylpropane.
-CH ₃ corr (quaternary)	A correction for the attachment of each methyl group to a quaternary carbon atom. Example: 2,2-Dimethylpropane.
-CH ₃ corr (tert/quat)	A correction for the attachment of each methyl group when there is both a tertiary and a quaternary carbon atom present in the longest chain of a hydrocarbon. Example: 2,2,3-Trimethylpentane.
-CH ₃ corr (quat/quat)	A correction for the attachment of each methyl group when there are two quaternary carbon atoms present in the longest chain of a hydrocarbon. Example: 2,2,4,4-Tetramethylpentane.
ortho corr, hydrocarbons	An aromatic ring correction for <i>ortho</i> substitution in hydrocarbon compounds. Example: o-Xylene.
meta corr, hydrocarbons	An aromatic ring correction for <i>meta</i> substitution in hydrocarbon compounds. Example: <i>m</i> -Xylene.
rsc	Ring strain correction, rsc, for a cyclic non-aromatic compound. Example: Cyclopropane.
rsc (unsub)	Ring strain correction, rsc, for a cyclic non-aromatic unsubstituted compound. Example: Cyclopentane.
rsc (sub)	Ring strain correction, rsc, for a cyclic non-aromatic substituted compound. Example: Methylcyclopentane.

TABLE 3. General definitions and examples of notations for organic groups - Continued

C (TT) (C)(C)	
C-(H) ₂ (C)(O)	A carbon atom bonded to two hydrogen atoms, a carbon atom, and an oxygen atom. Example: Methanol.
O-(C) ₂	An oxygen atom bonded to two carbon atoms. Example: Dimethyl ether.
C-(H)(O)(C) ₂ (alcohols, peroxides)	Tertiary carbon atom group in alcohols and peroxides. Example: 2-Propanol, n-Heptyl-2-hydroperoxide.
C-(H)(O)(C) ₂ (ethers, esters)	Tertiary carbon atom group in ethers and esters. Example: Methylisopropyl ether, Isopropyl acetate.
C-(O)(C) ₃ (alcohols, peroxides)	Quaternary carbon atom group in alcohols and peroxides. Example: tert-Butyl alcohol, Di-tert-butyl peroxide.
C-(O)(C) ₃ (ethers, esters)	Quaternary carbon atom group in ethers and esters. Example: Di-tert-butyl ether, tert-Butyl acctate.
C-(H) ₂ (C)(CN)	A carbon atom bonded to two hydrogen atoms, a carbon atom, and a nitrile (cyano) group. Example: Propanenitrile.
CB-(NO ₂)(CB) ₂	An aromatic ring carbon atom bonded to a nitro group and two other aromatic ring carbon atoms. Example: Nitrobenzene.
NO ₂ -NO ₂ (ortho corr)	A correction for adjacent (ortho) substitution of NO ₂ groups on an aromatic ring. Example: o-Dintrobenzene.
NO ₂ -COOH (ortho corr)	A correction for substitution of an NO ₂ group adjacent to a COOH group on an aromatic ring. Example: o-Nitrobenzoic acid.
N-(H) ₂ (C) (first, amino acids)	The first (and only) NH ₂ group bonded to a carbon atom in an amino acid. Example: Glycine
N-(H) ₂ (C) (second, amino acids)	The second NH_2 group bonded to a carbon atom in an amino acid. Example: Lysine
N-(H) ₂ (CO) (amides, ureas)	A NH ₂ group bonded to a carbonyl group, CO, in amides and ureas. Example: Acetamide, Urea.
N-(H) ₂ (CO) (amino acids)	A NH ₂ group bonded to a carbonyl group, CO, in amino acids. Example: Asparagine
N-(H)(C)(CO) (amides, ureas)	A NH group bonded to a hydrogen atom, carbon atom, and a carbonyl group in amides and ureas. Example: N-Methylformamide, Methylurea.
N-(H)(C)(CO) (amino acids)	A NH group bonded to a hydrogen atom, carbon atom, and a carbonyl group in amino acids. Example: Glycylglycine.
Zwitterion energy, aliphatic	A correction for the conversion of an amino acid or to a zwitterion in amino acids and peptides with aliphatic moieties. Example: Glycine, Glycylalanine.
Zwitterion energy, aromatic I	A correction for the conversion of an aromatic amino acid or peptide to a zwitterion containing an aromatic ring attached directly to a conjugation detering group (such as a -CH ₂ - group). Example: Phenylalanine, Glycylphenylalanine.
Zwitterion energy, aromatic II	A correction for the conversion of an aromatic amino acid or peptide to a zwitterion containing an aromatic ring attached directly to a conjugation enhancing group (such as a >C=O group). Example: Hippuric acid, Hippurylglycine.

TABLE 3. General definitions and examples of notations for organic groups - Continued

N _A -(C)	A doubly-bonded (azo) nitrogen atom bonded to a carbon atom. Example: Azomethane.
N_A - (C_B)	A doubly-bonded (azo) nitrogen atom bonded to an aromatic ring carbon atom. Example: trans-Azobenzene.
N _A -(oxide)(C)	A doubly-bonded (azoxy) nitrogen atom bonded to a carbon atom. Example: Di-tert-butyldiazene N-oxide
N _r -(C)	A doubly-bonded (imino) nitrogen atom bonded to a carbon atom. Example: N-Butylisobutyleneimine.
N_I – (C_B)	A doubly-bonded (pyridine-type) nitrogen atom bonded to an aromatic ring carbon atom. Example: Pyridine.
N _I -(CH ₃) (ortho corr)	A doubly-bonded (pyridine-type) nitrogen atom in an aromatic ring adjacent to a substituted methyl group. Example: 2-Picoline
N _I -N _I (ortho corr)	A doubly-bonded (pyridine-type) nitrogen atom adjacent to an identical (pyridine-type) nitrogen atom in an aromatic ring. Example: Pyridazine
C-(H) ₂ (C)(S)	A carbon atom bonded to two hydrogen atoms, a carbon atom, and a sulfur atom. Example: Methanethiol.
S-(C)(S)	A sulfur atom bonded to a carbon atom and another sulfur atom. Example: Dimethyl disulfide.
C-(H) ₂ (C)(F)	A carbon atom bonded to two hydrogen atoms, a carbon atom, and a fluorine atom. Example: Fluoroethane.
ortho corr, (F)(F)	A correction for the adjacent (ortho) substitution of two fluorine atoms on an aromatic ring. Example: o-Difluorobenzene.
ortho corr, (I)(COOH)	A correction for the substitution of a iodine atom adjacent (ortho) to a COOH group on an aromatic ring. Example: 2-iodobenzoic acid.
ortho corr (Cl)(Cl')	A correction for the substitution of a chlorine atom in an aromatic ring in the near proximity of another chlorine atom in a different aromatic ring which is bonded to the first ring. Example: 2,2'-Dichlorobiphenyl

TABLE 4. n-Alkanes (25)

TABLE 4. n-Alkanes (25) - Continued

Methane (1 × C(H	l) ₄), σ = 12	2		СН4	Pentane (2×C-(F	H) ₃ (C))+(3	×C-(H) ₂ (C) ₂),	, σ = 18	C ₅ H ₁₂
	Literatur	e – Calculated =	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $ \Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = $	-74.48 35.71 186.27	-74.48 35.73 186.26 -80.62 -50.44 20.35	0.00 -0.02 0.01	72PIT/PIL 89FRI/ELY 89FRI/ELY	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 146.82 120.21 348.95	- 146.41 120.13 348.09 - 464.04 - 8.06 3.25	- 0.41 0.08 0.86	70GOO 69STU/WES 69STU/WES
Ethane (1×2×C	C−(H)₃(C)), Literatur	σ = 18 re – Calculated =	= Residual	C₂H ₆ Reference	Liquid phase $ \Delta_{\ell}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{\ell}S^{\circ} = \Delta_{\ell}G^{\circ} = C_{p}^{\circ} = C_{p}^{\circ} = C_{p}^{\circ} = C_{p}^{\circ} $	se - 173.51 167.19 263.47	- 172.41 164.22 263.74 - 548.39 - 8.91	-1.10 2.97 -0.27	70GOO 67MES/GUT 67MES/GUT
Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	- 83.85 52.47 229.12	-83.85 52.63 229.49 -173.71 -32.06 12.93	0.00 -0.16 -0.37	72PIT/PIL 73CHA/WIL 73CHA/WIL	$\frac{\ln K_{\rm f}}{\rm Hexane}$ $(2 \times C - (F_{\rm f}))$		3.59 \times C-(H) ₂ (C) ₂), re – Calculated		C₅H₃. Reference
		×C-(H) ₂ (C) ₂), re – Calculated		C₃H ₈ Reference	Gas phase $\Delta_{l}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{l}S^{\circ} = \Delta_{l}G^{\circ} = \ln K_{l} = 0$	- 167.28 143.09 388.40	- 167.04 143.02 387.25 - 561.19 0.28 - 0.11	- 0.24 0.07 1.15	47OSB/GIN 69STU/WES 69STU/WES
Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	-104.68 73.60 270.20	- 105.15 74.35 269.77 - 269.74 - 24.73 9.98	0.47 - 0.75 0.43	72PIT/PIL 73CHA/WIL 73CHA/WIL	Liquid phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se 198.66 194.97 296.06	- 198.14 194.64 296.12 - 652.32 - 3.65 1.47	- 0.52 0.33 - 0.06	69GOO/SMI 46DOU/HUF 46DOU/HUF
Butane (2×C-(l	, , ,, ,	2×C-(H) ₂ (C) ₂),		C ₄ H ₁₀	Heptane	I) (CI) ((5		10	C ₇ H ₁₆
	Literatu	re – Calculated	= Kesiduai	Reference	(2×C-(F		\times C-(H) ₂ (C) ₂), re – Calculated		Reference
Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{1}{2}$	-125.65 98.49 309.91	-125.78 97.24 308.93 -366.89 -16.39 6.61	0.13 1.25 0.98	72PIT/PIL 75CHE/WIL 75CHE/WIL	Gas phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	187.48 165.98 427.90	187.67 165.91 426.41 658.34 8.61 3.47	0.19 0.07 1.49	47OSB/GIN 69STU/WES 69STU/WES

TABLE 4. n-Alkanes (25) - Continued

TABLE 4. n-Alkanes (25) - Continued

Heptane (C (2×C-(1		× C-(H) ₂ (C) ₂),	, σ = 18	C7H16	Decane (2×C-	(H)₃(C))+(8	8×C-(H) ₂ (C) ₂)	$\sigma = 18$	C ₁₆ H ₂
•	Literatur	e – Calculated	= Residual Re	ference		Literatu	re – Calculated	= Residual	Reference
Liquid pha Δ _i H° =	use - 224.05	- 223.87	-0.18	44PRO/ROS	Gas phase $\Delta_t H^\circ =$	- 249.66	- 249.56	-0.10	47OSB/GIN
$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = 0$	224.93 328.57	225.06 328.50 -756.25 1.61	-0.13 -0.07	61HUF/GRO 61HUF/GRO	$C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = S^{\circ}$	234.60 544.63	234.58 543.89 - 949.79 33.62	0.02 0.74	69STU/WES 69STU/WES
$lnK_f =$		- 0.65			$lnK_f =$		-13.56		
Octane (2×C-(1	H)3(C))+(6	× C-(H)2(C)2)	, σ = 18	C ₈ H ₁₈	Liquid ph $ \Delta_t H^\circ = \\ C_p^\circ = \\ S^\theta = \\ $	ase - 300.62 314.47 425.89	-301.06 316.32 425.64	0.44 -1.85 0.25	44PRO/ROS 54FIN/GRO2 54FIN/GRO2
	Literatur	e – Calculated	= Residual	Reference	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-1068.04 17.38 -7.01		
Gas phase $\Delta_t H^\circ = C_p^\circ =$	-208.27 188.87	-208.30 188.80	0.03 0.07	47OSB/GIN 69STU/WES			- 7.01		
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \Delta_t G^{\circ$	466.73	465.57 - 755.49 16.95	1.16	69STU/WES	Undecane (2×C-($9 \times C - (H)_2(C)_2$, σ = 18	C11H2
$ \Delta_f G^{\circ} = \\ \ln K_f = \\ $		- 6.84				Literatu	re – Calculated	= Residual	Reference
Liquid pha		040.60	0.10	44DD 0/D 00	Gas phase		270.10	0.50	4577 0 77 0 00
$\Delta_i H^\circ =$	- 249.78	-249.60	-0.18	44PRO/ROS	$\Delta_{\rm f}H^{\circ} =$	-270.91	-270.19	-0.72	45PRO/ROS2
$C_p^{\circ} = S^{\circ} =$	254.14 361.20	255.48 360.88	- 1.34 0.32	54FIN/GRO2	$C_p^{\circ} = S^{\circ} =$	257.44 583.58	257.47	-0.03	69STU/WES
_	301.20		0.32	54FIN/GRO2	$\Delta_{t}S^{\circ} =$	383.38	583.05	0.53	69STU/WES
$\Delta_{\rm f} S^{\circ} =$		-860.18					- 1046.94		
$\Delta_t G^\circ = \ln K_t =$		6.86 -2.77			$\Delta_f G^\circ = \ln K_f =$		41.96 16.92		
					Liquid ph				
Nonane (2×C-(H)3(C))+(7	× C-(H) ₂ (C) ₂)	$\sigma = 18$	C ₉ H ₂₀	$\Delta_t H^\circ = C_p^\circ = S^\circ =$	- 326.60 345.05 458.15	- 326.79 346.74 458.02	0.19 1.69 0.13	45PRO/ROS2 54FIN/GRO2 54FIN/GRO2
	Literatur	e – Calculated	= Residual	Reference	$\Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} =$		- 1171.97 22.63	3113	<i>3.</i>
Gas phase		228.02	0.60	47OCDICINI	$lnK_f =$	·····	- 9.13		
$\Delta_{\rm f}H^{\circ} =$	-228.24	-228.93	0.69	47OSB/GIN					
$C_p^{\circ} =$	211.71	211.69	0.02	69STU/WES	n. J				~
S° = Δ ₀ S° =	505.68	504.73 852.64	0.95	69STU/WES	Dodecane	TI) (C)) + (4	0.40 (11) (0)	10	$C_{12}H_{26}$
$\Delta_{t}G^{\circ} =$		-832.64 25.29			(2×0-(11/3(U)) + (I	0×C-(H) ₂ (C) ₂), cr = 18	
$\ln K_{\rm f} =$		- 10.20				Literatu	re – Calculated	= Residual	Reference
Liquid pha	ase		- marility Vanis		Gas phase $\Delta_t H^\circ =$	- 290.87	- 290.82	-0.05	45PRO/ROS2
$\Delta_t H^\circ =$	- 274.68	-275.33	0.65	69GOO	$C_p^{\circ} =$	280.33	280.36	-0.03	69STU/WES
$C_p^{\circ} =$	284.39	285.90	-1.51	54FIN/GRO2	$S^{\circ} =$	622.50	622.21	0.29	69STU/WES
S° =	393.67	393.26	0.41	54FIN/GRO2	$\Delta_{i}S^{\circ} =$	024.50	- 1144.10	V-4,3	03310/WE3
$\Delta_f S^\circ =$		-964.11			$\Delta_f G^\circ =$		50.29		
		12.12			$\ln K_{\rm f} =$		-20.29		
$\Delta_t G^{\circ} =$									

TABLE 4. n-Alkanes (25) - Continued

TABLE 4. n-Alkanes (25) - Continued

	Continued) 1) ₃ (C)) + (10	0×C-(H) ₂ (C) ₂)	, σ = 18	$C_{12}H_{26}$	Pentadecar (2×C-(J		3×C-(H) ₂ (C) ₂), σ = 18	C ₁₅ H ₃
	Literatur	e – Calculated :	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid pha	Se.				Gas phase				
$\Delta_{i}H^{\circ} =$	-352.13	-352.52	0.39	45PRO/ROS2	$\Delta_t H^\circ =$	-352.75	-352.71	~ 0.04	45PRO/ROS2
$C_p^{\circ} =$	375.97	377.16	-1.19	54FIN/GRO2	$C_p^{\circ} =$	348.95	349.03	-0.08	69STU/WES
$S^{\circ} =$	490.66	490.40	0.26	54FIN/GRO2	S° =	739.35	739.69	-0.34	69STU/WES
$\Delta_f S^\circ =$	470.00	- 1275.90	0.20	Janyonoz	$\Delta_{t}S^{\circ} =$	103.00	- 1435.55	0.54	0,010,1120
$\Delta_{\rm f}G^{\circ} =$		27.89			$\Delta_{\rm f}G^{\circ} =$		75.30		
$\ln K_{\rm f} =$		-11.25			$\ln K_{\rm f} =$		-30.37		
					Liquid pha	.ca			
Tridecane				СЧ	$\Delta_i H^\circ =$	- 428.82	- 429.71	0.89	ASDD O/D OS3
	U\ (C\\) (1	1 v C (II) (C) '	10	$C_{13}H_{28}$	•	469.95	468.42	1.53	45PRO/ROS2
(2 × C-()	n)3(C))+(1	$1 \times C - (H)_2(C)_2$), G = 18		$C_p^{\circ} = S^{\circ} =$				54FIN/GRO2
	T :44	ro Colout-4- 1	- Dockder-1	Doforces	$S^{\circ} = \Delta_{f}S^{\circ} =$	587.52	587.54 1597.70	-0.02	54FIN/GRO2
	Literatu	re – Calculated	– Residuai	Reference	-		1587.70		
					$\Delta_f G^\circ = \ln K_f =$		43.66 17.61		
Gas phase	044.70	946 15	0.05	45DD C 77 C 22	<u> </u>				
$\Delta_{\rm f}H^{\circ} =$	-311.50	-311.45	-0.05	45PRO/ROS2					
$C_p^{\circ} =$	303.21	303.25	-0.04	69STU/WES					
S° =	661.45	661.37	0.08	69STU/WES	Hexadecan				C ₁₆ H
$\Delta_f S^\circ =$		- 1241.25			(2×C-(1	H)₃(C))+(1	$14 \times C - (H)_2(C)_2$), $\sigma = 18$	
$\Delta_{\rm f}G^{\circ} =$		58.63							
$lnK_f =$		- 23.65				Literatu	re – Calculated	= Residual	Reference
					Gas phase				
Liquid pha	ise				$\Delta_f H^\circ =$	- 374.76	-373.34	-1.42	72MOR
$\Delta_i H^\circ =$	- 377.69	- 378.25	0.56	45PRO/ROS2	$C_{\rho}^{\circ} =$	371.79	371.92	- 0.13	69STU/WES
$C_p^{\circ} =$	406.89	407.58	-0.69	54FIN/GRO2	S° =	778.31	778.85	- 0.54	69STU/WES
S° =	522.87	522.78	0.09	54FIN/GRO2	$\Delta_{\mathbf{f}}S^{\circ} =$		1532.70		
$\Delta_{\mathbf{f}}S^{\circ} =$		- 1379.83			$\Delta_{\rm f}G^{\circ} =$		- 83.63		
$\Delta_f G^\circ =$		33.15			$lnK_f =$		-33.74		
$lnK_f =$		- 13.37							
		**************************************			Liquid pha	ise			
					$\Delta_{\ell}H^{\circ} =$	-456.14	- 455.44	-0.70	55FRA/PRO
Tetradecar	ne			C14H30	$C_{\rho}^{\circ} =$	501.45	498.84	2.61	54FIN/GRO2
(2×C-($H)_{3}(C)) + (1$	$2 \times C - (H)_2(C)_2$	$\sigma = 18$		s° =	619.65	619.92	-0.27	54FIN/GRO2
· - ·		- (/2(-/2	,,		$\Delta_f S^\circ =$		- 1691.63		
	Literatu	re - Calculated	= Residual	Reference	$\Delta_l G^{\circ} =$		48.92		
		····			$lnK_f =$		-19.73		
Gas phase					-				
$\Delta_{\rm f}H^{\circ} =$	-332.13	-332.08	-0.05	45PRO/ROS2	Solid phase	2			
$C_p^{\circ} =$	326.06	326.14	-0.08	69STU/WES	$\Delta_t H^\circ =$	- 507.50	-505.22	-2.28	69STU/WES
S° =	700.40	700.53	-0.13	69STU/WES	$C_p^{\circ} =$	441.79	441.78	0.01	
$\Delta_{t}S^{\circ} =$. 00.70	- 1338.40	0.15	0.020,1100	$S^{\circ} =$	434.84	435.52	-0.68	
$\Delta_{\rm f}G^{\circ} =$		66.96			$\Delta_{f}S^{\circ} =$	101101	- 1876.03	0.00	
$\ln K_{\rm f} =$		- 27.01			$\Delta_{\rm f}G^{\circ} =$		54.12		
		۵/.UI			$\ln K_f =$		-21.83		
Liquid -L	are.								
Liquid phate $\Delta_i H^\circ =$	– 403.25	-403.98	0.73	45PRO/ROS2					
$C_p^{\circ} =$	438.44	438.00	0.44	54FIN/GRO2					
	555.43	555.16	0.27	54FIN/GRO2					
	JJJ.7J		0.21	J41 114/ONO2					
S° =		~ 1481./h							
$S^{\circ} = \Delta_{t}S^{\circ} =$		1483.76 38 40							
S° =		- 1483.76 38.40 - 15.49							

TABLE 4. n-Alkanes (25) - Continued

TABLE 4. n-Alkanes (25) - Continued

Heptadecan (2×C-(H		5×C-(H)2(C)2)), σ = 18	C ₁₇ H ₃₆	Nonadecar (2×C-(17×C-(H) ₂ (C)	$_2$), $\sigma = 18$	C19H4
	Literatur	re – Calculated	= Residual	Reference		Literatu	re – Calculated	l = Residual	Reference
Gas phase					Gas phase				
$\Delta_{\mathbf{f}}H^{\circ} =$	-393.92	- 393.97	0.05	45PRO/ROS2	$\Delta_{\rm f}H^{\circ} =$	-435.14	- 435.23	0.09	45PRO/ROS2
$C_p^{\circ} =$	394.68	394.81	-0.13	69STU/WES	$C_p^* =$	440.41	440.59	-0.18	69STU/WES
S° =	817.26	818.01	-0.75	69STU/WES	$S^{\circ} = \Delta_{f}S^{\circ} =$	895.17	896.33	-1.16	69STU/WES
$\Delta_{\rm f} S^{\circ} =$		- 1629.85			$\Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} =$		- 1824.15 108.64		
$\Delta_f G^\circ = \ln K_f =$		91.97 - 37.10			$\ln K_{\rm f} =$		- 43.83		
		- 37.10					45.05		
Liquid phas					Liquid pha				
_	-479.86	- 481.17	1.31	45PRO/ROS2	$\Delta_l H^{\circ} =$	- 530.95	-532.63	1.68	45PRO/ROS2
$C_p^{\circ} =$	534.34	529.26	5.08	67MES/GUT	$C_p^{\circ} =$		590.10		
S° =	652.24	652.30	-0.06	67MES/GUT	S° = Δ _t S° =		717.06		
$\Delta_f S^\circ = \Delta_f G^\circ =$		- 1795.56 54.18			$\Delta_{\mathbf{f}} S^{\circ} = \Delta_{\mathbf{f}} G^{\circ} = 0$		- 2003,42 64,69		
$lnK_f =$		-21.85			$\ln K_{\rm f} =$		-26.10		
						-			
Solid phase					Solid phas	e			
•	- 530.97	- 534.63	3.66	67MES/GUT	$\Delta_t H^\circ =$		-593.45		
$C_p^{\circ} =$		463.70			$C_p^{\circ} =$		507.54		
S° =		458.53			S° =		504.55		
$\Delta_f S^\circ =$		- 1989.33			$\Delta_f S^\circ = \Delta_f G^\circ =$		- 2215.93 67.23		
		58.49							
$\Delta_f G^\circ = In K_\circ =$		_ 23 59			$\ln K_c =$		27 12		
$\ln K_{\rm f} =$	· · · · · · · · · · · · · · · · · · ·	-23.59	·		$lnK_f =$		-27.12		
InK _f =) $\alpha = 18$	C ₁₈ H ₃₈	Eicosane	H) ₂ (C)) + (1		a) a = 18	C ₂₀ H ₄₂
InK _f =	· I)₃(C))+(1	16×C-(H)2(C)2			Eicosane	, , ,, ,	18×C-(H) ₂ (C);	•	
InK _f =	· I)₃(C))+(1			C ₁₈ H ₃₈	Eicosane	, , ,, ,		•	C ₂₀ H ₄₂ Reference
Octadecane (2×C-(H	H)₃(C)) + (1 Literatu	16×C-(H)2(C)2 re – Calculated	= Residual	Reference	Eicosane (2×C-(Literatu	18×C-(H) ₂ (C); re – Calculated	= Residual	Reference
$lnK_t =$ Octadecane $(2 \times C - (H))$ Gas phase $\Delta_t H^\circ =$	H)₃(C)) + (1 Literatu -414.55	16 × C-(H) ₂ (C) ₂ re - Calculated - 414.60	= Residual	Reference 45PRO/ROS2	Eicosane $(2 \times C - (1))$ Gas phase $\Delta_t H^\circ =$	Literatu -455.76	18×C-(H) ₂ (C); re – Calculated – 455.86	= Residual	Reference 45PRO/ROS2
$\begin{array}{c} \ln K_t = \\ \hline \\ \text{Octadecane} \\ (2 \times \text{C-(I)} \\ \hline \\ \text{Gas phase} \\ \Delta_t H^\circ = \\ C_p^\circ = \\ \end{array}$	H) ₃ (C)) + (1 Literatu -414.55 417.56	16 × C-(H) ₂ (C) ₂ re Calculated 414.60 417.70	= Residual 0.05 - 0.14	Reference 45PRO/ROS2 69STU/WES	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_p^\circ = 0$	Literatu - 455.76 463.29	18 × C-(H) ₂ (C); ore - Calculated - 455.86 463.48	0.10 -0.19	Reference 45PRO/ROS2 69STU/WES
Octadecane $(2 \times C - (F))$ Gas phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = C_p^{\circ} = C_p^{\circ}$	H)₃(C)) + (1 Literatu -414.55	16 × C-(H) ₂ (C) ₂ re - Calculated -414.60 417.70 857.17	= Residual	Reference 45PRO/ROS2	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = $	Literatu -455.76	18 × C-(H) ₂ (C); are - Calculated - 455.86 463.48 935.49	= Residual	Reference 45PRO/ROS2
Octadecane $(2 \times C - (F + G + G))$ Gas phase $\Delta_{L}H^{\circ} = C_{P}^{\circ} = S^{\circ} = \Delta_{L}S^{\circ} = C_{L}G^{\circ}$	H) ₃ (C)) + (1 Literatu -414.55 417.56	16 × C-(H) ₂ (C) ₂ re - Calculated - 414.60 417.70 857.17 - 1727.00	= Residual 0.05 - 0.14	Reference 45PRO/ROS2 69STU/WES	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = 0$	Literatu - 455.76 463.29	18 × C-(H) ₂ (C) ₂ re - Calculated - 455.86 463.48 935.49 - 1921.30	0.10 -0.19	Reference 45PRO/ROS2 69STU/WES
Octadecane $(2 \times C - (F))$ Gas phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = C_p^{\circ} = C_p^{\circ}$	H) ₃ (C)) + (1 Literatu -414.55 417.56	16 × C-(H) ₂ (C) ₂ re - Calculated -414.60 417.70 857.17	= Residual 0.05 - 0.14	Reference 45PRO/ROS2 69STU/WES	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = $	Literatu - 455.76 463.29	18 × C-(H) ₂ (C); are - Calculated - 455.86 463.48 935.49	0.10 -0.19	Reference 45PRO/ROS2 69STU/WES
In K_f = Octadecane (2 × C-(F) Gas phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_f = InK_f$	-414.55 417.56 856.21	-414.60 417.70 857.17 -1727.00 100.31	= Residual 0.05 - 0.14	Reference 45PRO/ROS2 69STU/WES	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t = InK_t$	- 455.76 463.29 934.12	18 × C-(H) ₂ (C) ₂ re - Calculated - 455.86 463.48 935.49 - 1921.30 116.98	0.10 -0.19	Reference 45PRO/ROS2 69STU/WES
In K_f = Octadecane (2 × C-(H Gas phase $\Delta_t H^\circ =$ $C_t^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ In $K_f =$ Liquid phase	-414.55 417.56 856.21	-414.60 417.70 857.17 -1727.00 100.31 -40.46	0.05 -0.14 -0.96	45PRO/ROS2 69STU/WES 69STU/WES	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t = InK_t$ Liquid pha	- 455.76 463.29 934.12	-455.86 463.48 935.49 -1921.30 116.98 -47.19	0.10 - 0.19 - 1.37	Reference 45PRO/ROS2 69STU/WES 69STU/WES
In K_t = Octadecane (2 × C-(H Gas phase $\Delta_t H^\circ =$ $C_t^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ In $K_t =$ Liquid phase $\Delta_t H^\circ =$	-414.55 417.56 856.21	-414.60 417.70 857.17 -1727.00 100.31 -40.46	= Residual 0.05 - 0.14	Reference 45PRO/ROS2 69STU/WES	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{2}$ Liquid pha $\Delta_t H^\circ = \frac{1}{2}$	- 455.76 463.29 934.12	-455.86 463.48 935.49 -1921.30 116.98 -47.19	0.10 -0.19	Reference 45PRO/ROS2 69STU/WES
Octadecane $(2 \times C - (H \cup Gas))$ Gas phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t G^\circ = InK_t = InK_t = InK_t = C_t^\circ = C_t^\circ = C_t^\circ = InK_t^\circ = C_t^\circ = InK_t^\circ = C_t^\circ = InK_t^\circ = InK_t^\circ = InK_t^\circ = C_t^\circ = InK_t^\circ = InK_t$	-414.55 417.56 856.21	-414.60 417.70 857.17 -1727.00 100.31 -40.46	0.05 -0.14 -0.96	45PRO/ROS2 69STU/WES 69STU/WES	Eicosane $(2 \times C - f)$ Gas phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{2}$ Liquid pha $\Delta_t H^\circ = C_t^\circ = \frac{1}{2}$	- 455.76 463.29 934.12	-455.86 463.48 935.49 -1921.30 116.98 -47.19	0.10 - 0.19 - 1.37	Reference 45PRO/ROS2 69STU/WES 69STU/WES
Octadecane $(2 \times C - (I \times C)^{\circ})$ Gas phase $\Delta_{t}H^{\circ} = C_{t}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = InK_{t} = InK_{t}$ Liquid phase $\Delta_{t}H^{\circ} = C_{t}^{\circ} = S^{\circ} = S^{\circ} = S^{\circ} = S^{\circ} = S^{\circ} = S^{\circ} = S^{\circ}$	-414.55 417.56 856.21	-414.60 417.70 857.17 -1727.00 100.31 -40.46	0.05 -0.14 -0.96	45PRO/ROS2 69STU/WES 69STU/WES	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{2}$ Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \frac{1}{2}$	- 455.76 463.29 934.12	-455.86 463.48 935.49 -1921.30 116.98 -47.19	0.10 - 0.19 - 1.37	Reference 45PRO/ROS2 69STU/WES 69STU/WES
In K_f = Octadecane (2 × C-(F) Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_f = \frac{\Delta_t H^\circ}{\Delta_t H^\circ} = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ}{\Delta_t S^\circ} = \frac{\Delta_t S^\circ}$	-414.55 417.56 856.21	-414.60 417.70 857.17 -1727.00 100.31 -40.46 -506.90 559.68 684.68 -1899.49	0.05 -0.14 -0.96	45PRO/ROS2 69STU/WES 69STU/WES	Eicosane $(2 \times C - f)$ Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ}{\Delta_t H^\circ} = \frac{C_\rho^\circ}{S^\circ} = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ}{\Delta_t S^\circ} = \Delta_t S^\circ$	- 455.76 463.29 934.12	-455.86 463.48 935.49 -1921.30 116.98 -47.19 -558.36 620.52 749.44 -2107.35	0.10 - 0.19 - 1.37	Reference 45PRO/ROS2 69STU/WES 69STU/WES
Octadecane $(2 \times C - (I \times C)^{\circ})$ Gas phase $\Delta_{t}H^{\circ} = C_{t}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = InK_{t} = InK_{t}$ Liquid phase $\Delta_{t}H^{\circ} = C_{t}^{\circ} = S^{\circ} = S^{\circ} = S^{\circ} = S^{\circ} = S^{\circ} = S^{\circ} = S^{\circ}$	-414.55 417.56 856.21	-414.60 417.70 857.17 -1727.00 100.31 -40.46	0.05 -0.14 -0.96	45PRO/ROS2 69STU/WES 69STU/WES	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{2}$ Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \frac{1}{2}$	- 455.76 463.29 934.12	-455.86 463.48 935.49 -1921.30 116.98 -47.19	0.10 - 0.19 - 1.37	Reference 45PRO/ROS2 69STU/WES 69STU/WES
In K_f = Octadecane (2 × C – (F Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = InK_f = InK_f$	-414.55 417.56 856.21	-414.60 417.70 857.17 -1727.00 100.31 -40.46 -506.90 559.68 684.68 -1899.49 59.43	0.05 -0.14 -0.96	45PRO/ROS2 69STU/WES 69STU/WES	Eicosane $(2 \times C - (1)^{-1})$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = InK_t = In$	- 455.76 463.29 934.12	-455.86 463.48 935.49 -1921.30 116.98 -47.19 -558.36 620.52 749.44 -2107.35 69.95	0.10 - 0.19 - 1.37	Reference 45PRO/ROS2 69STU/WES 69STU/WES
In $K_t =$ Octadecane $(2 \times C - (H \times G)^{\circ})$ Gas phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t G^{\circ} = InK_t =$ Liquid phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t G^{\circ} = InK_t =$ Solid phase	-414.55 417.56 856.21	-414.60 417.70 857.17 -1727.00 100.31 -40.46 -596.80 559.68 684.68 -1899.49 59.43 -23.97	0.05 - 0.14 - 0.96	Reference 45PRO/ROS2 69STU/WES 69STU/WES 45PRO/ROS2	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = InK_t = In$	- 455.76 463.29 934.12	- 455.86 463.48 935.49 - 1921.30 116.98 - 47.19 - 558.36 620.52 749.44 - 2107.35 69.95 - 28.22	0.10 - 0.19 - 1.37	Reference 45PRO/ROS2 69STU/WES 69STU/WES
In K_t = Octadecane (2×C-(H Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ In $K_t =$ Liquid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t G^\circ =$	-414.55 417.56 856.21	-414.60 417.70 857.17 -1727.00 100.31 -40.46 -506.90 559.68 684.68 -1899.49 59.43 -23.97	-3.10	Reference 45PRO/ROS2 69STU/WES 69STU/WES 45PRO/ROS2	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t}{2}$ Liquid phase $\Delta_t H^\circ = \frac{C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t}{2}$ Solid phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t G^\circ = S^\circ = \Delta_t G^\circ = S^\circ = \Delta_t G^\circ = S^\circ = S$	- 455.76 463.29 934.12	-455.86 463.48 935.49 -1921.30 116.98 -47.19 -558.36 620.52 749.44 -2107.35 69.95 -28.22	0.10 -0.19 -1.37	Reference 45PRO/ROS2 69STU/WES 69STU/WES 45PRO/ROS2
In $K_t =$ Octadecane $(2 \times C - (H \times G)^{\circ})$ Gas phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t G^{\circ} = InK_t =$ Liquid phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t G^{\circ} = InK_t =$ Solid phase	-414.55 417.56 856.21 se -505.43	-414.60 417.70 857.17 -1727.00 100.31 -40.46 -506.90 559.68 684.68 -1899.49 59.43 -23.97	-3.10 0.05 -0.14 -0.96	45PRO/ROS2 69STU/WES 69STU/WES 45PRO/ROS2 67MES/GUT 67MES/GUT	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = InK_t = In$	- 455.76 463.29 934.12	-455.86 463.48 935.49 -1921.30 116.98 -47.19 -558.36 620.52 749.44 -2107.35 69.95 -28.22	0.10 -0.19 -1.37	Reference 45PRO/ROS2 69STU/WES 69STU/WES 45PRO/ROS2
In K_f = Octadecane (2 × C-(H Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t G^\circ =$ In $K_f =$ Liquid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ In $K_f =$ Solid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$	-414.55 417.56 856.21	-414.60 417.70 857.17 -1727.00 100.31 -40.46 -506.90 559.68 684.68 -1899.49 59.43 -23.97	-3.10	Reference 45PRO/ROS2 69STU/WES 69STU/WES 45PRO/ROS2	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{C_p^\circ = S^\circ = $	- 455.76 463.29 934.12	-455.86 463.48 935.49 -1921.30 116.98 -47.19 -558.36 620.52 749.44 -2107.35 69.95 -28.22	0.10 -0.19 -1.37	Reference 45PRO/ROS2 69STU/WES 69STU/WES 45PRO/ROS2
In K_t = Octadecane (2×C-(H Gas phase $\Delta_t H^\circ =$ $C_r^\circ =$ $S^\circ =$ $\Delta_t G^\circ =$ In $K_t =$ Liquid phase $\Delta_t H^\circ =$ $C_r^\circ =$ $S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Solid phase $\Delta_t H^\circ =$ $C_r^\circ =$	-414.55 417.56 856.21 se -505.43	-414.60 417.70 857.17 -1727.00 100.31 -40.46 -506.90 559.68 684.68 -1899.49 59.43 -23.97	-3.10 0.05 -0.14 -0.96	45PRO/ROS2 69STU/WES 69STU/WES 45PRO/ROS2 67MES/GUT 67MES/GUT	Eicosane $(2 \times C - (1))^{-1}$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = InK_t = In$	- 455.76 463.29 934.12	-455.86 463.48 935.49 -1921.30 116.98 -47.19 -558.36 620.52 749.44 -2107.35 69.95 -28.22	0.10 -0.19 -1.37	Reference 45PRO/ROS2 69STU/WES 69STU/WES 45PRO/ROS2

TABLE 4. n-Alkanes (25) - Continued

TABLE 4. n-Alkanes (25) - Continued

Tetracosane (2×C-(H		\times C-(H) ₂ (C) ₂)	C24H50	Hexacosan (2×C-(1		$24 \times C - (H)_2(C)_2$)	C ₂₆ H ₅
	Literature	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
····					Gas phase				
Gas phase					$\Delta_{\mathbf{f}}H^{\circ} =$		- 579.64		
$\Delta_t H^{\circ} =$		-538.38			$C_p^{\circ} =$		600.82		
$C_p^{\circ} =$		555.04				· · · · · · · ·			
					Liquid pha	se			
Liquid phas	е				$\Delta_{\mathbf{f}}H^{\circ} =$		-712.74		
$\Delta_t H^\circ =$		-661.28			$C_p^{\circ} =$		803.04		
$C_p^{\circ} =$		742.20			<i>s</i> ° =		943.72		
S° =		878.96			$\Delta_f S^\circ =$		-2730.94		
Δ _i S° =		-2523.07			$\Delta_{\rm f}G^{\circ} =$		101.49		
$\Delta_{f}G^{\circ} =$		90.97			$\ln K_{\rm f} =$		40.94		
$\ln K_{\rm f} =$		- 36.70							
					Solid phase	.			
Solid phase					$\Delta_t H^{\circ} =$	•	- 799.32		
$\Delta_{\rm f}H^{\circ} =$		- 740.50			$C_p^{\circ} =$	661.20	660.98	0.22	76AND/MAR
$C_p^{\circ} =$	730.94	617.14	113.80	49PAR/MOO	$S^{\circ} =$	667.01	665.62	1.39	-
$S^{\circ} =$	651.03	619.60				007.01		1.39	76AND/MAR
$\Delta_{f}S^{\circ} =$	031.03		31.43	49PAR/MOO	$\Delta_{f}S^{\circ} =$		- 3009.04		
$\Delta_{\mathbf{f}} S^{\circ} =$		-2782.44			$\Delta_t G^{\circ} =$		97.82		
$\Delta_{\mathbf{f}}G^{\circ} =$		89.08			$lnK_f =$		- 39.46		
$lnK_f =$		- 35.94							
		-35.94		<u> </u>	Dotrigeont	ane.			СЧ
lnK _f =				C ₂₅ H ₅₂	Dotriacont: (2×C-(I		30×C-(H)2(C)2		C ₃₂ H ₆
lnK _f =		-35.94 3×C-(H) ₂ (C) ₂)	C ₂₅ H ₅₂		I)₃(C))+(3			
lnK _f =	I) ₃ (C)) + (23			C ₂₅ H ₅₂		I)₃(C))+(3	30 × C-(H)2(C)2 re – Calculated		C ₃₂ H ₄ Reference
lnK _f =	I) ₃ (C)) + (23	3×C-(H) ₂ (C) ₂			(2×C-(I	I)₃(C))+(3			
InK _f = Pentacosan (2×C-(H	I) ₃ (C)) + (23	3×C-(H) ₂ (C) ₂			(2×C-(I	I)₃(C))+(3	re – Calculated		
Pentacosan (2×C-(H	I) ₃ (C)) + (23	3×C−(H)₂(C)₂ e − Calculated			$(2 \times C - (I))$ Gas phase $\Delta_t H^\circ =$	I)₃(C))+(3	re – Calculated – 703.42		
InK _f = Pentacosan (2 × C-(H	I) ₃ (C)) + (23	3×C-(H) ₂ (C) ₂			(2×C-(I	I)₃(C))+(3	re – Calculated		
$\begin{aligned} & \ln K_{\rm f} = \\ & \text{Pentacosam} \\ & (2 \times \text{C-(H)} \\ & \text{Gas phase} \\ & \Delta_{\rm f} H^{\circ} = \end{aligned}$	I) ₃ (C)) + (23	$3 \times C - (H)_2(C)_2$ e – Calculated – 559.01			Gas phase $\Delta_t H^{\circ} = C_p^{\circ} =$	H)₃(C))+(3 Literatu	re – Calculated – 703.42		
In K_f = Pentacosam (2 × C-(H Gas phase $\Delta_t H^\circ = C_p^\circ =$	() ₃ (C)) + (23	$3 \times C - (H)_2(C)_2$ e – Calculated – 559.01			$(2 \times C - (I - I))$ Gas phase $\Delta_t H^\circ = C_p^\circ = $	H)₃(C))+(3 Literatu	- 703.42 738.16		
In K_f = Pentacosan (2×C-(H Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase	() ₃ (C)) + (23	3 × C-(H) ₂ (C) ₂ e – Calculated – 559.01 577.93			$(2 \times C - (I - I))$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid pha $\Delta_t H^\circ =$	H)₃(C))+(3 Literatu	- 703.42 738.16		
In K_f = Pentacosand (2 × C-(H Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ =$	() ₃ (C)) + (23	3 × C-(H) ₂ (C) ₂ e - Calculated - 559.01 577.93			Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid pha $\Delta_t H^\circ = C_p^\circ =$	H)₃(C))+(3 Literatu	- 703.42 738.16 - 867.12 985.56		
In K_f = Pentacosane (2 × C-(H Gas phase $\Delta_t H^\circ = C_\rho^\circ =$ Liquid phas $\Delta_t H^\circ = C_\rho^\circ =$	() ₃ (C)) + (23	3 × C-(H) ₂ (C) ₂ e - Calculated - 559.01 577.93 - 687.01 772.62			Gas phase $\Delta_t H^\circ = C_p^\circ = {}$ Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = {}$	H)₃(C))+(3 Literatu	- 703.42 738.16 - 867.12 985.56 1138.00		
Pentacosam $(2 \times C - (H + G))^2$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p^\circ$	() ₃ (C)) + (23	3×C-(H) ₂ (C) ₂ e - Calculated - 559.01 577.93 - 687.01 772.62 911.34			Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ Liquid pha $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ $S_{p}^{\circ} = $ $\Delta_{t}S^{\circ} = $	H)₃(C))+(3 Literatu	- 703.42 738.16 - 867.12 985.56 1138.00 - 3354.52		
Pentacosam $(2 \times C - (H + G + G))$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p$	() ₃ (C)) + (23	3×C-(H) ₂ (C) ₂ e - Calculated - 559.01 577.93 - 687.01 772.62 911.34 - 2627.01			Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid pha $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} =$	H)₃(C))+(3 Literatu	-703.42 738.16 -867.12 985.56 1138.00 -3354.52 133.03		
Pentacosam $(2 \times C - (H))$ Gas phase $\Delta_{l}H^{\circ} = C_{p}^{\circ} =$ Liquid phas $\Delta_{l}H^{\circ} = C_{p}^{\circ} =$ $S^{\circ} =$	() ₃ (C)) + (23	3×C-(H) ₂ (C) ₂ e - Calculated - 559.01 577.93 - 687.01 772.62 911.34			Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ Liquid pha $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ $S_{p}^{\circ} = $ $\Delta_{t}S^{\circ} = $	H)₃(C))+(3 Literatu	- 703.42 738.16 - 867.12 985.56 1138.00 - 3354.52		
Pentacosam $(2 \times C - (H + G + G))$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p$	() ₃ (C)) + (23	- 559.01 577.93 - 687.01 772.62 911.34 - 2627.01 96.23			Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{1}{2}$ Liquid pha $\Delta_t H^\circ = C_p^\circ = \frac{1}{2}$ $\Delta_t S^\circ = \Delta_t S^\circ = \frac{1}{2}$ $\Delta_t G^\circ = \frac{1}{2}$	H)₃(C))+(3 Literatu	-703.42 738.16 -867.12 985.56 1138.00 -3354.52 133.03		
In K_f = Pentacosam (2 × C-(H) Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phas $\Delta_t H^\circ = S_p^\circ =$ $\Delta_t S_p^\circ = \Delta_t S_p^\circ =$ In $K_f =$	() ₃ (C)) + (23 Literatur	- 559.01 577.93 - 687.01 772.62 911.34 - 2627.01 96.23			Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid pha $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = InK_{t} =$ Solid phase	H)₃(C))+(3 Literatu	- 703.42 738.16 - 867.12 985.56 1138.00 - 3354.52 133.03 - 53.66	= Residual	Reference
In K_f = Pentacosam (2 × C-(H) Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = \Delta_t G^\circ = \ln K_f =$ Solid phase	() ₃ (C)) + (23 Literatur	-559.01 577.93 -687.01 772.62 911.34 -2627.01 96.23 -38.82			Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid pha $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $S^{\circ} = \Delta_{t}S^{\circ} =$ $\ln K_{t} =$ Solid phase $\Delta_{t}H^{\circ} =$	H)₃(C))+(3 Literatu	- 703.42 738.16 - 867.12 985.56 1138.00 - 3354.52 133.03 - 53.66	= Residual	Reference 31BEC
In K_f = Pentacosam (2 × C-(H Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = S_p^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ In $K_f =$ Solid phase $\Delta_t H^\circ =$	I) ₃ (C)) + (23 Literatur	-559.01 577.93 -687.01 772.62 911.34 -2627.01 96.23 -38.82	= Residual	Reference	Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ = \ln K_t =$ Solid phase $\Delta_t H^\circ = C_p^\circ =$ $C_p^\circ = C_p^\circ =$	H ₃ (C))+(3 Literatu Literatu - 968.34 877.38	- 703.42 738.16 - 867.12 985.56 1138.00 - 3354.52 133.03 - 53.66	7.44 84.88	Reference 31BEC 49PAR/MOO
In K_f = Pentacosam (2 × C-(H Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ In $K_f =$ Solid phase $\Delta_t H^\circ =$ $C_p^\circ =$	() ₃ (C)) + (23 Literatur ee	-559.01 577.93 -687.01 772.62 911.34 -2627.01 96.23 -38.82 -769.91 639.06	= Residual	Reference 30PAR/HUF	Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{1}{2}$ Liquid pha $\Delta_t H^\circ = C_p^\circ = \frac{1}{2}$ $\Delta_t S^\circ = \frac{1}{2}$ Arso = $\frac{1}{2}$ Solid phase $\Delta_t H^\circ = \frac{1}{2}$ $\Delta_t H^\circ = \frac{1}{2}$ Solid phase $\Delta_t H^\circ = \frac{1}{2}$ $\Delta_t H^\circ = \frac{1}{2}$ Solid phase	H)₃(C))+(3 Literatu	- 703.42 738.16 - 867.12 985.56 1138.00 - 3354.52 133.03 - 53.66 - 975.78 792.50 803.68	= Residual	Reference 31BEC
In K_f = Pentacosam (2 × C-(H) Gas phase $\Delta_t H^\circ = C_p^\circ = C_p^\circ = Liquid phase$ $\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = L_t S^$	I) ₃ (C)) + (23 Literatur	-559.01 577.93 -687.01 772.62 911.34 -2627.01 96.23 -38.82 -769.91 639.06 642.61	= Residual	Reference	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{S^{\circ}}{S^{\circ}} = \frac{S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{S^{\circ}}{S^{\circ}} = S$	H ₃ (C))+(3 Literatu Literatu - 968.34 877.38	- 703.42 738.16 - 867.12 985.56 1138.00 - 3354.52 133.03 - 53.66 - 975.78 792.50 803.68 - 3688.84	7.44 84.88	Reference 31BEC 49PAR/MOO
In K_f = Pentacosam (2 × C-(H) Gas phase $\Delta_t H^\circ = C_p^\circ = C_p^\circ = Liquid phase$ $\Delta_t H^\circ = C_p^\circ = Liquid phase$ $\Delta_t G^\circ = Liquid phase$	() ₃ (C)) + (23 Literatur ee	- 559.01 577.93 - 687.01 772.62 911.34 - 2627.01 96.23 - 38.82 - 769.91 639.06 642.61 - 2895.74	= Residual	Reference 30PAR/HUF	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \frac{C_{p}^{\circ}}{C_{p}^{\circ}} = \frac{C_{p}$	H ₃ (C))+(3 Literatu Literatu - 968.34 877.38	- 703.42 738.16 - 867.12 985.56 1138.00 - 3354.52 133.03 - 53.66 - 975.78 792.50 803.68 - 3688.84 124.05	7.44 84.88	Reference 31BEC 49PAR/MOO
In K_f = Pentacosam (2 × C-(H) Gas phase $\Delta_t H^\circ = C_p^\circ = C_p^\circ = Liquid phase$ $\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = L_t S^$	() ₃ (C)) + (23 Literatur ee	-559.01 577.93 -687.01 772.62 911.34 -2627.01 96.23 -38.82 -769.91 639.06 642.61	= Residual	Reference 30PAR/HUF	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{\Delta_{t}H^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{S^{\circ}}{S^{\circ}} = \frac{S^{\circ}}{S^$	H ₃ (C))+(3 Literatu Literatu - 968.34 877.38	- 703.42 738.16 - 867.12 985.56 1138.00 - 3354.52 133.03 - 53.66 - 975.78 792.50 803.68 - 3688.84	7.44 84.88	Reference 31BEC 49PAR/MOO

TABLE 4. n-Alkanes (25) - Continued

TABLE 5. t-Alkanes	(35)	١
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	TABLE 4	n-Alkanes (2	25) — Conti	nued	***************************************		TABLE 5. t-Al	kanes (35)	
Tritriaconta (2×C-(H		1×C-(H) ₂ (C) ₂))	C ₃₃ H ₆₈		$H_{3}(C) + (1$	$1 \times C - (H)(C)_3$ (Liary)), $\sigma = 81$	+	C ₄ H ₁₀
***************************************	Literatu	re – Calculated :	= Residual	Reference	(5 ^ C1	·	re – Calculated	= Residual	Reference
Gas phase					•		···		<u></u>
$\Delta_t H^\circ =$		-724.05			Gas Phase				
$C_p^{\circ} =$		761.05			$\Delta_f H^\circ =$	-134.18	-134.73	0.55	72PIT/PIL
•					$C_{\rho}^{\circ} =$	96.65	97.27	-0.62	75CHE/WIL
					<i>S</i> ° =	295.39	291.82	3.57	75CHE/WIL
Liquid phas	e				$\Delta_{\epsilon}S^{\circ} =$		-383.99		
$\Delta_{\mathbf{f}}H^{\circ} =$		-892.85			$\Delta_{\rm f}G^{\circ} =$		-20.24		
$C_p^{\circ} =$		1015.98			$lnK_{\ell} =$		8.17		
s° =		1170.38							·····
$\Delta_{\mathbf{f}}S^{\circ} =$		-3458.45							
$\Delta_f G^\circ =$		138.29							
$lnK_f =$		- 55.78			2-Methylbu	utane			C5H12
					(3×C-(1	$H)_3(C)) + (1$	\times C-(H) ₂ (C) ₂)	$+(1\times C-(H)($	$(C)_3) +$
					(2×-CF	I₃ corr (tert	iary)), $\sigma = 27$		
Solid phase									
$\Delta_{\rm f}H^{\circ} =$		-1005.19		***		Literatu	re – Calculated	= Residual	Reference
$C_p^{\circ} =$	900.82	814.42	86.40	30PAR/HUF					
S° =	877.80	826.69	51,11	30PAR/HUF	G 51				
$\Delta_{\rm f}S^{\circ} =$		-3802.14			Gas Phase		150.10	0.45	
$\Delta_l G^{\circ} =$		128.42			$\Delta_{\rm f}H^{\circ} =$	-152.93	-153.10	0.17	70GOO
$lnK_{\ell} =$		-51.80			$C_p^{\circ} = S^{\circ} =$	118.78	120.16	-1.38	69STU/WES
					$\Delta_t S^\circ =$	343.59	340.12	3.47	69STU/WES
					$\Delta_{\rm f}G^{\circ} =$		-472.01		
							- 12.37		
					$\ln K_{\rm f} =$		4.99		
					Liquid Pha				
					$\Delta_{\rm f}H^{\circ} =$	- 178.91	-177.69	-1.22	70GOO
					$C_p^{\circ} =$	164.85	161.24	3.61	43GUT/HUF
					S° =	260.41	258.39	2.02	43GUT/HUF
					$\Delta_f S^\circ =$		- 553.74		
					$\Delta_{\rm f}G^{\circ} =$		- 12.59		
					$lnK_f =$	······	5.08		
					2-Methylpe (3×C-(1 (2×-CH	$H)_3(C)) + (2$	\times C-(H) ₂ (C) ₂) iary)), $\sigma = 27$	+ (1 × C-(H)(C ₆ H ₁₄
						Literatu	re – Calculated	= Residual	Reference
					Gas Phase	487			
					$\Delta_{f}H^{\circ} =$	-174.77	- 173.73	-1.04	49WAD/SMI
					$C_p^{\circ} =$	144.18	143.05	1.13	69STU/WES
					S° =	380.53	379.28	1.25	69STU/WES
					$\Delta_t S^\circ =$		-569.16		
					$\Delta_i G^\circ =$		-4.03		
					$lnK_f =$		1.63		
					Liquid Pha		005 ::		
					$\Delta_i H^\circ =$	- 204.64	-203.42	-1.22	41PRO/ROS
					$C_p^{\circ} =$	193.72	191.66	2.06	46DOU/HUF
					S° =	290.58	290.77	-0.19	46DOU/HUF
					$\Delta_f S^\circ =$		- 657.67		
					$\Delta_t G^\circ =$		-7.34 2.06		
					$lnK_f =$		2.96		

TABLE 5. t-Alkanes (35) - Continued

TABLE 5. t-Alkanes (35) - Continued

	Literatur	e – Calculated :	= Residual	Reference		Literatu	ire – Calculated	= Residual	Reference
Gas phase	, ,				Liquid pha	se			
Δ ₁ H° =	- 194.64	- 194.36	-0.28	86TRC	$\Delta_{\mathbf{f}}H^{\circ} =$		-280.61		
$C_p^{\circ} =$	165.98	165.94	0.04	69STU/WES	$C_p^{\circ} =$		282.92		
S° =	419.99	418.44	1.55	69STU/WES	S° =		387.91		
$\Delta_f S^\circ =$		-666.31			$\Delta_{f}S^{\circ} =$		- 969.46		
$\Delta_{\rm f}G^{\circ} =$		4.30			$\Delta_{\mathbf{f}}G^{\circ} =$		8.43		
$lnK_f =$		-1.73		•	$\ln K_{\rm f} =$		-3.40		
Liquid phas	se			•	2-Methylno	nane			C ₁₀ H
$\Delta_t H^\circ =$	- 229.49	-229.15	-0.34	41PRO/PRS2	(3×C-(1	$H)_3(C)) + (0)$	$6 \times C - (H)_2(C)_2)$	+ (1 × C-(H)(C) ₃) +
$C_p^{\circ} =$	222.92	222.08	0.84	61HUF/GRO	(2×-CH	l ₃ corr (ter	tiary)), $\sigma = 27$		
S° =	323.34	323.15	0.19	61HUF/GRO					
$\Delta_f S^\circ =$		- 761.60				Literatu	ire – Calculated	= Residual	Reference
$\Delta_i G^{\circ} =$		-2.08							
$lnK_f =$		0.84			a 1				
					Gas phase $\Delta_t H^\circ =$		-256.25		
					$C_p^{\circ} =$	242.09	234.61	7.48	69STU/WES
2-Methylhe	ntone			C ₈ H ₁₈	S° =	534.46	535.92	- 1.46	69STU/WES
		\times C-(H) ₂ (C) ₂)	+ (1 × C-(H)($\Delta_{f}S^{\circ} =$		-957.76	20	0,010,1120
		iary)), $\sigma = 27$	(= ()(-707	$\Delta_t G^{\circ} =$		29.31		
`	` `	****			$lnK_f =$		-11.82		
	Literatu	re – Calculated	= Residual	Reference					
Can abase					Liquid pha $\Delta_t H^\circ =$	se	-306.34		
Gas phase $\Delta_t H^\circ =$	-215.35	- 214.99	-0.36	47OSB/GIN	$C_p^{\circ} =$	313.30	- 306.34 313.34	- 0.04	41PAR/WES
$C_p^{\circ} =$	188.87	188.83	0.04	69STU/WES	S° =	420.07	420.29	-0.22	41PAR/WES
S° =	455.26	457.60	-2.34	69STU/WES	$\Delta_f S^\circ =$		- 1073.39	0.22	
$\Delta_f S^\circ =$		-763.46		.,	$\Delta_{\mathfrak{l}}G^{\circ} =$		13.69		
$\Delta_f G^{\circ} =$		12.64			$lnK_f =$		-5.52		
$lnK_f =$		-5.10							
Liquid pha	se				2-Methylde	cane			C ₁₁ H
$\Delta_t H^\circ =$	-255.01	-254.88	-0.13	45PRO/ROS	(3×C-(I	H) ₃ (C))+('	$7 \times C - (H)_2(C)_2$	+ (1 × C-(H)(
$C_p^{\circ} =$	252.00	252.50	-0.50	71MES/FIN	(2×-CH	l ₃ corr (ter	tiary))		
S° =	356.39	355.53	0.86	71MES/FIN					
$\Delta_f S^\circ =$		-865.53				Literatu	ire – Calculated	= Residual	Reference
$\Delta_f G^\circ =$		3.18						144	
$lnK_f =$		-1.28			Gos mboso				
					Gas phase $\Delta_f H^\circ =$		-276.88		
					$C_p^{\circ} =$		257.50		
2-Methyloc	tane			C ₉ H ₂₀			231.30		
		$5 \times C - (H)_2(C)_2$	+ (1×C-(H)(
		iary)), $\sigma = 27$	` ` ` ` ` `	, ,-,	Liquid pha	se			
	•				$\Delta_f H^{\circ} =$		-332.07		
	Literatu	re – Calculated	= Residual	Reference	$C_p^{\circ} =$	341.21	343.76	-2.55	71MES/FIN
					S° =	453.80	452.67	1.13	71MES/FIN
					$\Delta_{\mathbf{f}}S^{\circ} =$		- 1177.32		
Gas phase					$\Delta_{\mathbf{f}}G^{\circ} =$		18.95		
$\Delta_t H^\circ =$	045.05	-235.62		(00mm: =====	$lnK_f =$		−7.64		
$C_p^{\circ} =$	217.07	211.72	5.35	69STU/WES					
S° =	495.89	496.76	-0.87	69STU/WES					
$\Delta_f S^\circ =$		-860.61							
		20.97							
$\Delta_f G^\circ = \ln K_f =$		- 8.46							

TABLE 5. t-Alkanes (35) - Continued

	$H)_3(C)) + (2$	\times C-(H) ₂ (C) ₂) iary)), $\sigma = 54$	+ (1 × C-(H)(C ₆ H ₁₄	(3×C-(ntinued) $4 \times C - (H)_2(C)_2$ tiary)), $\sigma = 27$		C ₈ H ₁₆ (C) ₃)+
	Literatu	re – Calculated	= Residual	Reference		Literatu	ire – Calculated	l = Residual	Reference
Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	-172.09 143.09 379.78	-171.47 143.05 373.51 -574.92 -0.06	-0.62 0.04 6.27	49WAD/SMI 69STU/WES 69STU/WES	Liquid pha $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	252.34 250.20 362.63	- 252.70 252.50 355.53 - 865.53 5.36	0.36 -2.30 7.10	45PRO/ROS 73FIN/MES 73FIN/MES
$\ln K_f =$		0.02			$lnK_f =$		-2.16		
Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = A_s S^\circ $	-202.38 190.66 292.55	-201.24 191.66 290.77 -657.67	-1.14 -1.00 1.78	41PRO/ROS 73MES/FIN 73MES/FIN		H) ₃ (C)) + (5	$5 \times C - (H)_2(C)_2$ tiary)), $\sigma = 27$,		C ₉ H ₂₀ (C) ₃) +
$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-5.16 2.08				Literatu	re – Calculated	= Residual	Reference
	H)3(C))+(3 I3 corr (tert	\times C-(H) ₂ (C) ₂) iary)), $\sigma = 27$, re – Calculated	$\eta = 2$	C ₇ H ₁₆ C) ₃) + Reference	Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	212.59 501.66	-233.36 211.72 502.52 -854.85 21.51 -8.68	0.87 - 0.86	69STU/WES 69STU/WES
Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	-191.33 165.98 424.13	- 192.10 165.94 424.20 - 660.55 4.84 - 1.95	0.77 0.04 - 0.07	86TRC 69STU/WES 69STU/WES	Liquid pha $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se	-278.43 282.92 387.91 -969.46 10.61 -4.28		
Liquid pha $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	- 226.44 218.00 309.60	- 226.97 222.08 323.15 - 761.60 0.10 - 0.04	0.53 -4.08 -13.55	41PRO/ROS2 30HUF/PAR2 30HUF/PAR2		H)3(C))+(6 3 corr (tert	$\sigma \times C - (H)_2(C)_2$ iary)), $\sigma = 27$, re – Calculated	$\eta = 2$	C ₁₆ H ₂₂ C) ₃) + Reference
	H) ₃ (C)) + (4 I ₃ corr (tert	×C-(H) ₂ (C) ₂) iary)), σ = 27, re – Calculated	$\eta = 2$	C ₈ H ₁₈ C) ₃)+ Reference	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_f = 0$	237.61 540.24	- 253,99 234.61 541.68 - 952.00 29.85 - 12.04	3.00 - 1.44	69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-212.51 188.87 461.58	- 212.73 188.83 463.36 - 757.70 13.18 - 5.32	0.22 0.04 - 1.78	47OSB/GIN 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	308.99 427.19	-304.16 313.34 420.29 -1073.39 15.87 -6.40	-4.35 6.90	41PAR/WES 41PAR/WES

TABLE 5. t-Alkanes (35) - Continued

TABLE 5. t-Alkanes (35) - Continued

	I)₃(C))+(4:	\times C-(H) ₂ (C) ₂) - ary)), $\sigma = 54$	- (1×C-(H)(C ₈ H ₁₈		$H)_3(C)) + (6$	finued) $6 \times C - (H)_2(C)_2$ iary)), $\sigma = 27$,		C ₁₀ H ₂ (C) ₃) +
	Literatur	e – Calculated =	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	-211.96 188.87	-212.73 188.83	0.77 0.04	47OSB/GIN 69STU/WES	Liquid pha $ \Delta_t H^\circ = C_p^\circ = $	se 317.36	-304.16 313.34	4.02	41PAR/WES
$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$	453.34	451.83 - 769.23 16.61 - 6.70	1.51	69STU/WES	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$	425.51	420.29 - 1073.39 15.87 - 6.40	5.22	41PAR/WES
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = 0$	se - 251.63 251.09	-252.70 252.50 355.53 -865.53	1.07 -1.41	45PRO/ROS 47OSB/GIN		H) ₃ (C))+(6	$5 \times C - (H)_2(C)_2$ iary)), $\sigma = 54$	+ (1×C-(H)(C ₁₀ H (C) ₃)+
$\Delta_f G^\circ = \\ \ln K_f =$		5.36 -2.16				Literatu	re – Calculated	= Residual	Reference
	····			Attention	Gas phase $\Delta_t H^\circ =$		-253.99		
	$H_{3}(C)) + (5$	\times C-(H) ₂ (C) ₂) iary)), $\sigma = 27$,		C ₉ H ₂₀ C) ₃)+	$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = 0$	237.61 534.46	234.61 530.15 - 963.53 33.29	3.00 4.31	69STU/WES 69STU/WES
-	Literatu	re – Calculated	= Residual	Reference	$lnK_f =$		-13.43		
Gas phase $\Delta_t H^\circ =$		-233.36			Liquid pha $\Delta_t H^\circ =$		-304.16		
$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f = 0$	212.59 501.66	211.72 502.52 -854.85 21.51 -8.68	0.87 -0.86	69STU/WES 69STU/WES	$C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$	314.43 423.84	313.34 420.29 - 1073.39 15.87 - 6.40	1.09 3.55	41PAR/WES 41PAR/WES
Liquid pha	se		,					· · · · · · · · · · · · · · · · · · ·	
$\Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} =$		-278.43 282.92 387.91			3-Ethylpen (3×C-(1		×C-(H) ₂ (C) ₂)	+ (1×C-(H)(C_7H_1 $(C)_3), \sigma = 54$
$\Delta_f S^\circ = \Delta_f G^\circ =$		- 969.46 10.61				Literatu	re – Calculated	= Residual	Reference
$\ln K_{\rm f} =$		-4.28			Gas phase $\Delta_{\mathbf{f}}H^{\circ} = C_{p}^{\circ} =$	-189.33 165.98	189.84 165.94	0.51 0.04	47OSB/GIN 69STU/WES
	H) ₃ (C)) + (6	$i \times C - (H)_2(C)_2$ iary)), $\sigma = 27$,		C ₁₀ H ₂₂ C) ₃) +	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$	411.50	412.67 - 672.07 10.54 - 4.25	-1.17	69STU/WES
	Literatu	re – Calculated	= Residual	Reference			-		
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	237.61 540.24	-253.99 234.61 541.68 -952.00 29.85	3.00 -1.44	69STU/WES 69STU/WES	Liquid pha $ \Delta_t H^\circ = \\ C_p^\circ = \\ S^\circ = \\ \Delta_t S^\circ = \\ \Delta_t G^\circ = \\ \ln K_f - \\ $	- 224.56 219.58 314.55	- 224.79 222.08 323.15 - 761.60 2.28 - 0.92	0.23 -2.50 -8.60	41PRO/ROS2 61HUF/GRO 61HUF/GRO

ESTIMATION OF THERMODYNAMIC PROPERTIES OF ORGANIC COMPOUNDS

3-Ethylhexa	ane			C ₈ H ₁₈	3-Ethylocta	ne (Contin	ued)		C ₁₀ H
		\times C-(H) ₂ (C) ₂)	+ (1 × C-(H)((3×C-(1	$H)_3(C)) + (6$	\times C-(H) ₂ (C) ₂)	$+(1\times C-(H)($	
	Literatui	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gos aboss					Liquid pha	S.P.			
Gas phase $\Delta_t H^\circ =$	-210.71	-210.47	-0.24	47OSB/GIN	$\Delta_t H^\circ =$.50	-301.98		
$C_p^{\circ} =$	188.87	188.83	0.04	69STU/WES	$C_{\rho}^{\circ} =$		313.34		
S° =	458.19	457.60	0.59	69STU/WES	<i>s</i> ° =		420.29		
$\Delta_{\mathbf{f}}S^{\circ} =$		-763.46			$\Delta_{\mathbf{f}}S^{\circ} =$		- 1073.39		
$\Delta_i G^{\circ} =$		17.16			$\Delta_f G^{\circ} =$	•	18.05		
$lnK_f =$		-6.92			$lnK_f =$		-7.28		
Liquid pha	se								
$\Delta_{f}H^{\circ} =$	-250.41	-250.52	0.11	45PRO/ROS	4-Ethylhep			4.	C ₉ H ₂
$C_p^{\circ} =$		252.50			$(3 \times C - (1 \times C - (1 \times C + (1 \times C) + (1 \times C + (1 \times C) + (1 \times C + (1 \times C) + $	H)₃(C))+(5	\times C-(H) ₂ (C) ₂)	$+(1\times C-(H)($	$C)_3), \sigma = 54$
S° =		355.53				T			D
$\Delta_f S^\circ =$		-865.53				Literatu	re – Calculated	= Residual	Reference
$\Delta_{\rm f}G^{\circ} =$		7.54							
$lnK_f =$		-3.04			Gos mharr				
					Gas phase $\Delta_t H^\circ =$		-231.10		
					$C_p^{\circ} =$	208.11	- 231.10 211.72	-3.61	COSTI LAMES
2 Fabriles	4			C ₉ H ₂₀	$S^{\circ} =$	495.89	490.99	- 3.61 4.90	69STU/WES
3-Ethylhep		~C (II) (C))	LANC (H)		$\Delta_f S^\circ =$	493.09	- 866.38	4.90	69STU/WES
(3×C-()	13(0))+(3	\times C-(H) ₂ (C) ₂)	T(17C-(H)($C_{J3J}, U = 2I$	$\Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} =$		- 806.38 27.21		
	I itaratu	re – Calculated	= Residual	Reference	$\ln K_{\rm f} =$		- 10.98		
	Literatu		= Kesiuuai	Reference			- 10.96		
Gas phase					Liquid pha	se			
$\Delta_t H^\circ =$		-231.10			$\Delta_{f}H^{\circ} =$		- 276.25		
$C_p^{\circ} =$	208.11	211.72	-3.61	69STU/WES	$C_p^{\circ} =$		282.92		
S° =	495.89	496.76	-0.87	69STU/WES	S° =		387.91		
$\Delta_f S^\circ =$		-860.61			$\Delta_{f}S^{\circ} =$		-969.46		
$\Delta_{\mathfrak{c}}G^{\circ} =$		25.49			$\Delta_t G^{\circ} =$		12.79		
$\ln K_{\rm f} =$		- 10.28			$lnK_f =$		-5.16		
Liquid pha	se								
$\Delta_{\rm f}H^{\circ} =$		-276.25			4-Ethylocta				C10H2
$C_r^{\circ} =$		282.92			(3×C-(F	1)₃(C))+(6:	\times C-(H) ₂ (C) ₂)	+(1×C-(H)(0	$\Gamma(s)_3$), $\sigma = 27$, $\eta = 1$
S° =		387.91				T 1.			
$\Delta_f S^\circ =$		-969.46				Literatui	re – Calculated	= Residual	Reference
$\Delta_i G^{\circ} =$		12.79							
$lnK_f =$		-5.16			Gos nhas-				
					Gas phase $\Delta_t H^\circ =$		-251.73		
					$C_p^{\circ} =$	233.13	- 231.73 234.61	-1.48	60CTI IAMES
3-Ethylocts	ne			C10H22	$S^{\circ} =$	534.46	541.68	- 1.48 - 7.22	69STU/WES 69STU/WES
		\times C-(H) ₂ (C) ₂)	+(1×C-(H)($\Delta_{f}S^{\circ} =$	J.74.4U	-952.00	- 1.22	0931U/WE3
(3 ^ 0-()	· • /3(~)/ T (U	~~(11)2(C)2))(11)-0 - (11)(C/3/, 0 - 21	Δ _i G° =		32.11		
	Literatu	re – Calculated	= Residual	Reference	$lnK_f =$		- 12.95		
Goo where		The second secon			Tionid at-	no.			
Gas phase		251 72			Liquid pha	SC	201.00		
$\Delta_i H^\circ =$	222.12	- 251.73	4.40	COCCUTATION	$\Delta_{\mathbf{f}}H^{\circ} =$		-301.98		
$C_{\nu}^{\circ} = S^{\circ} =$	233.13	234.61	1.48 1.46	69STU/WES	$C_{\mu}^{\circ} = S^{\circ} =$		313.34		
3° = Δ _t S° =	534.46	535.92 -957.76	- 1.40	69STU/WES	$\Delta_{f}S^{\circ} =$		420.29 1073.39		
$\Delta_{\mathbf{f}}G^{\circ} =$		33.83			$\Delta_{i}G^{\circ} =$				
$d_1G^* = d_1K_1 = d_1K_2$		33.83 13.65					18.05 7.28		
					InK. =				

- 13.65

 $lnK_f =$

-7.28

 $lnK_t =$

TABLE 5. t-Alkanes (35) - Continued

TABLE 5. t-Alkanes (35) - Continued

	Y 14.	Called 1	D - 22 - 1	D - C	$(4 \times -CH_3 \text{ corr (tertiary)}), \sigma = 162$				
	Literature	- Calculated =	- Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase									
$\Delta_i H^\circ =$	ы	-251.73			Liquid pha				
$C_p^{\circ} =$	233.13	234.61	- 1.48	69STU/WES	$\Delta_{\rm f}H^{\circ} =$	-234.60	- 234.43	-0.17	41PRO/ROS
s° =	525.34	530.15	-4.81	69STU/WES	$C_{\rho}^{\circ} =$	224.22	219.10	5.12	61HUF/GRO
$\Delta_{\mathbf{f}}S^{\circ} =$		-963.53			S° =	303.17	317.80	- 14.63	61HUF/GRO
$\Delta_{\mathbf{f}}G^{\circ} =$		35.55			$\Delta_{f}S^{\circ} =$		<i>−</i> 766.95		
$lnK_f =$		- 14.34			$\Delta_{\mathbf{f}}G^{\circ} = \ln K_{\mathbf{f}} =$		-5.76 2.33		
iquid phas	20					·····			
ndaio biis: γ:	, , , , , , , , , , , , , , , , , , ,	- 301.98							
$C_p^{\circ} =$		313.34			2,4-Dimeth	vlhexane			Cal
S° =		420.29					\times C-(H) ₂ (C) ₂)	+ (2 × C-(H)(
Δ ₆ S° =		-1073.39					iary)), $\sigma = 81$	(2/(0 (11)(C)3) 1
$\Delta_{\rm f}G^{\circ} =$		18.05			(37. 01)	., (1016			
$\ln K_{\rm f} =$		-7.28				Literatu	re – Calculated	= Residual	Reference
								1100	
-Isopropyl	heptane			$C_{10}H_{22}$	Gas phase $\Delta_t H^\circ =$	-219.24	-219.42	0.18	47OSB/GIN
		\times C-(H) ₂ (C) ₂)	+ (2×C-(H)($C_p^{\circ} =$	188.87	188.86	0.01	69STU/WES
(2×-CH	3 corr (tertia	$ary)), \sigma = 54$			<i>S</i> ° =	445.64	449.63	- 3.99	69STU/WES
·					$\Delta_{\mathbf{f}}S^{\circ} =$		−771.43		
	Literatur	e – Calculated:	= Residual	Reference	$\Delta_f G^{\circ} =$		10.58		
					$lnK_f =$		-4.27		
Gas phase									
$\Delta_t H^\circ =$		-258.42			Liquid pha				
$C_p^{\circ} =$	231.00	234.64	-3.64	69STU/WES	$\Delta_{\rm f}H^{\circ} =$	- 257.02	-257.98	0.96	45PRO/ROS
S° =	521.45	525.55	-4.10	69STU/WES	$C_p^{\circ} =$		249.52		
Δ _t S° =		-968.13			S° =		350.18		
$\Delta_{\mathbf{f}}G^{\circ} =$		30.23			$\Delta_{\mathbf{f}}S^{\circ} =$		-870.88		
$lnK_f =$		- 12.19			$\Delta_t G^\circ = \ln K_t =$		1.67 - 0.67		
iquid pha	se								
$\Delta_t H^\circ =$		-307.26							
		310.36			2,5-Dimeth	ylhexane			C ₈ F
$C_{p}^{\circ} =$		414.94			(4×C-(1	$H)_3(C)) + (2$	\times C-(H) ₂ (C) ₂)	$+(2\times C-(H)(0)$	C) ₃) +
$C_{P}^{\circ} = S^{\circ} =$		- 1078.74			(4×-CH	[3 corr (terti	$iary)$), $\sigma = 162$	2	
		1427							
$S^{\circ} = \Delta_{f}S^{\circ} =$		14.37						D 11 1	Reference
S° =		5.80				Literatu	re – Calculated	= Residual	
$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} =$			- Administra		Gas phase	Literatur	re – Calculated	= Kesidual	
$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$	vlnentane			C-H.	Gas phase				
$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = -\frac{1}{2}$	ylpentane H) ₃ (C)) + (1	- 5.80	+ (2 × C-(H)(C ₂ H ₁₆	$\Delta_t H^{\circ} =$	-222.51	- 221.68	-0.83	47OSB/GIN
$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f = \frac{1}{4}$.4-Dimeth	H) ₃ (C))+(1	-5.80 × C-(H) ₂ (C) ₂)			$\Delta_t H^\circ = C_p^\circ =$	-222.51 188.87	-221.68 188.86	-0.83 0.01	47OSB/GIN 69STU/WES
$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f = -\frac{1}{4}$ (4 × C-(1)	H) ₃ (C))+(1	- 5.80			$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} =$	-222.51	- 221.68 188.86 438.10	-0.83	47OSB/GIN
$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f = -\frac{1}{4}$ (4 × C-(1)	H) ₃ (C))+(1 I ₃ corr (terti	-5.80 × C-(H) ₂ (C) ₂)	2		$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} =$	-222.51 188.87	-221.68 188.86	-0.83 0.01	47OSB/GIN 69STU/WES
$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f = \frac{1}{4}$.4-Dimeth	H) ₃ (C))+(1 I ₃ corr (terti	-5.80 × C-(H) ₂ (C) ₂) ary)), $\sigma = 162$	2	C) ₃) +	$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} =$	-222.51 188.87	- 221.68 188.86 438.10 - 782.96	-0.83 0.01	47OSB/GIN 69STU/WES
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \ln K_t = \frac{2.4 \cdot \text{Dimeth}}{4 \times \text{C-(1)}}$ Gas phase	H) ₃ (C))+(1 I ₃ corr (terti Literatur	-5.80 × C-(H) ₂ (C) ₂) ary)), σ = 162 re - Calculated	= Residual	C) ₃) + Reference	$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1}{2}$	-222.51 188.87 439.03	- 221.68 188.86 438.10 - 782.96 11.76	-0.83 0.01	47OSB/GIN 69STU/WES
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \ln K_t = \frac{2.4 \cdot \text{Dimeth}}{4 \times \text{C-(1)}}$ Gas phase	H) ₃ (C))+(1 I ₃ corr (terti	-5.80 × C-(H) ₂ (C) ₂) ary)), $\sigma = 162$	2	C) ₃) +	$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = $ Liquid pha	- 222.51 188.87 439.03	- 221.68 188.86 438.10 - 782.96 11.76	-0.83 0.01 0.93	47OSB/GIN 69STU/WES 69STU/WES
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \ln K_t = \frac{4 \times C - (1 \times C - C)}{4 \times - C + C}$ Gas phase $\Delta_t H^{\circ} = C_p^{\circ} = \frac{4 \times C}{2}$	H) ₃ (C))+(1 I ₃ corr (terti Literatur	-5.80 × C-(H) ₂ (C) ₂) ary)), σ = 162 re - Calculated -201.05 165.97	= Residual	C) ₃) + Reference	$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = $ Liquid pha $\Delta_t H^{\circ} = $	-222.51 188.87 439.03	- 221.68 188.86 438.10 - 782.96 11.76 - 4.74	-0.83 0.01	47OSB/GIN 69STU/WES
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \ln K_t = -\frac{4}{4 \times C - (1)}$ Gas phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = -\frac{4}{3}$	H) ₃ (C)) + (1 I ₃ corr (terti Literatur -201.71	-5.80 × C-(H) ₂ (C) ₂) ary)), σ = 162 re - Calculated -201.05	= Residual - 0.66	Reference 47OSB/GIN	$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = $ Liquid pha	- 222.51 188.87 439.03	- 221.68 188.86 438.10 - 782.96 11.76 - 4.74 - 260.16 249.52	-0.83 0.01 0.93	47OSB/GIN 69STU/WES 69STU/WES
$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{4}{4}$ $A =$	H) ₃ (C))+(1 I ₃ corr (terti Literatur -201.71 165.98	-5.80 × C-(H) ₂ (C) ₂) ary)), σ = 162 re - Calculated -201.05 165.97	= Residual - 0.66 0.01	Reference 47OSB/GIN 69STU/WES	$\Delta_t H^{\circ} =$ $C_p^{\circ} =$ $S^{\circ} =$ $\Delta_t S^{\circ} =$ $\Delta_t G^{\circ} =$ $\ln K_t =$ Liquid pha $\Delta_t H^{\circ} =$ $C_p^{\circ} =$ $S^{\circ} =$	- 222.51 188.87 439.03	- 221.68 188.86 438.10 - 782.96 11.76 - 4.74	-0.83 0.01 0.93	47OSB/GIN 69STU/WES 69STU/WES 45PRO/ROS
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \ln K_t = \frac{2}{4}$. A.Dimeth $(4 \times C - (1 + 4 \times C + C))$. Gas phase $\Delta_t H^{\circ} = C_p^{\circ} = \frac{2}{4}$.	H) ₃ (C))+(1 I ₃ corr (terti Literatur -201.71 165.98	-5.80 × C-(H) ₂ (C) ₂) ary)), σ = 162 re - Calculated -201.05 165.97 398.94	= Residual - 0.66 0.01	Reference 47OSB/GIN 69STU/WES	$\Delta_t H^{\circ} =$ $C_p^{\circ} =$ $S^{\circ} =$ $\Delta_t S^{\circ} =$ $\Delta_t G^{\circ} =$ $\ln K_t =$ Liquid pha $\Delta_t H^{\circ} =$ $C_p^{\circ} =$	- 222.51 188.87 439.03	- 221.68 188.86 438.10 - 782.96 11.76 - 4.74 - 260.16 249.52	-0.83 0.01 0.93	47OSB/GIN 69STU/WES 69STU/WES 45PRO/ROS
$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \ln K_{t} = 0$ A-Dimeth $(4 \times C - (1) + (4 \times - CH)$ Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = 0$	H) ₃ (C))+(1 I ₃ corr (terti Literatur -201.71 165.98	-5.80 × C-(H) ₂ (C) ₂) ary)), σ = 162 re - Calculated -201.05 165.97 398.94 -685.81	= Residual - 0.66 0.01	Reference 47OSB/GIN 69STU/WES	$\Delta_t H^{\circ} =$ $C_p^{\circ} =$ $S^{\circ} =$ $\Delta_t S^{\circ} =$ $\Delta_t G^{\circ} =$ $\ln K_t =$ Liquid pha $\Delta_t H^{\circ} =$ $C_p^{\circ} =$ $S^{\circ} =$	- 222.51 188.87 439.03	- 221.68 188.86 438.10 - 782.96 11.76 - 4.74 - 260.16 249.52 350.18	-0.83 0.01 0.93	47OSB/GIN 69STU/WES 69STU/WES

TABLE 5. t-Alkanes (35) - Continued

TABLE 5. t-Alkanes (35) - Continued

	$H_{3}(C)) + (2$	\times C-(H)(C) ₃) + iary)), $\sigma = 162$		C ₆ H ₁₄		$H)_3(C)) + (2$	Continued) $\times C-(H)_2(C)_2$ iary)), $\sigma = 81$	+ (2×C-(H)(C ₈ H ₁₁
	Literatu	re – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t =$	- 178.28 140.54 365.77	-180.42 143.08 359.78 -588.66 -4.91 1.98	2.14 - 2.54 5.99	47OSB/GIN 69STU/WES 69STU/WES	Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	se - 252.59	- 257.98 249.52 350.18 - 870.88 1.67 - 0.67	5.39	45PRO/ROS
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = 0$	se 207.40	- 208.70 188.68 285.42 - 663.02	1.30	41PRO/ROS		$H)_3(C)) + (2$	\times C-(H) ₂ (C) ₂) iary)), $\sigma = 81$	+ (2×C-(H)(C ₈ H ₁₆ C) ₃) +
$\Delta_f G^\circ = \ln K_f =$		- 11.02 4.45				Literatu	re – Calculated	= Residual	Reference
	H) ₃ (C))+(1 I ₃ corr (tert	\times C-(H) ₂ (C) ₂) iary)), $\sigma = 81$ re – Calculated		C_7H_{16} $C)_3) +$ Reference	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t =$	-212.84 188.87 448.32	- 217.16 188.86 449.63 - 771.43 12.84 - 5.18	4.32 0.01 -1.31	47OSB/GIN 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_{t'}^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	198.87 165.98 414.05	- 198.79 165.97 410.47 - 674.28 2.25 - 0.91	-0.08 0.01 3.58	47OSB/GIN 69STU/WES 69STU/WES	Liquid pha $ \Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se - 251.83	- 255.80 249.52 350.18 - 870.88 3.85 - 1.55	3.97	45PRO/ROS
Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	- 233.09 218.30 297.10	- 232.25 219.10 317.80 - 766.95 - 3.58 1.45	- 0.84 - 0.80 - 20.70	41PRO/ROS2 76FIN/GRO 76FIN/GRO		H ₃ (C)) + (2 I ₃ corr (tert	ne \times C-(H) ₂ (C) ₂) iary)), $\sigma = 81$ $\sigma = -C$ alculated		C ₈ H ₁₈ C)3) + Reference
2,3-Dimeth (4 × C-(1	H) ₃ (C))+(2 I ₃ corr (tert	$2 \times C - (H)_2(C)_2$ iary)), $\sigma = 81$ re – Calculated		C ₈ H ₁₈ C) ₃) + Reference	Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	-211.04 188.87 441.12	- 217.16 188.86 443.86 - 777.20 14.56 - 5.87	6.12 0.01 - 2.74	47OSB/GIN 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 213.80 188.87 443.96	-219.42 188.86 443.86 -777.20 12.30 -4.96	5.62 0.01 0.10	47OSB/GIN 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	se 249.58	-255.80 249.52 350.18 -870.88 3.85 -1.55	6.22	45PRO/ROS

	TABLE S	5. t-Alkanes (35) – Contir	nued			Table 6. q-Al	kanes (16)		
(5×C-(e ×C-(H)(C) ₃)- iary)), σ = 243		C ₈ H ₁₈	2,2-Dimethylpropane $(4 \times C-(H)_3(C)) + (1 \times C-(C)_4) + (4 \times -CH_3 \text{ corr (quaternary))}, \sigma = 972$				C ₅ H ₁₂	
	Literatu	re – Calculated	= Residual	Reference		Literatu	re – Calculated	l = Residual	Reference	
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-217.32 188.87 428.07	- 226.11 188.89 430.13 - 790.93 9.71 - 3.92	8.79 - 0.02 - 2.06	47OSB/GIN 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 167.94 121.63 306.39	-168.08 119.45 302.59 -509.53 -16.16 6.52	0.14 2.18 3.80	70GOO 69STU/WES 69STU/WES	
Liquid ph $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	ase - 255.01 246.23 329.32	- 263.26 246.54 344.83 - 876.23 - 2.01 0.81	8.25 - 0.31 - 15.51	45PRO/ROS 41PIT/SCO 41PIT/SCO	Liquid pha $\Delta_{t}H^{\circ} =$ $C_{\rho}^{\circ} =$ $S^{\circ} =$ $\Delta_{t}S^{\circ} =$ $\Delta_{t}G^{\circ} =$ $\ln K_{t} =$	- 190.33 153.09 216.81	190.01 156.16 234.55 577.58 17.81 7.18	- 0.32 - 3.07 - 17.74	70GOO 69STU/WES 69STU/WES	
	(H)₃(C))+(4	$4 \times C - (H)_2(C)_2$ iary)), $\sigma = 16$		C ₁₀ H ₂₂		H)3(C))+(1 I3 corr (qua	ternary)), σ =			
	Literatu	re – Calculated	= Residual	Reference		Literatu	re – Calculated	l = Residual	Reference	
Gas phase $H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = 0$	e -264.01 235.56 515.68	- 262.94 234.64 516.42 - 977.26	-1.07 0.92 -0.74	69STU/WES 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	-186.10 141.88 358.23	- 184.15 142.34 353.28 - 595.16 - 6.70	- 1.95 - 0.46 4.95	47OSB/GIN 69STU/WES 69STU/WES	

	Literatu	Calculated	- Residuai	Reference
Gas phase	;			
H° =	-264.01	-262.94	-1.07	69STU/WES
$C_p^{\circ} =$	235.56	234.64	0.92	69STU/WES
s° =	515.68	516.42	-0.74	69STU/WES
$\Delta_f S^\circ =$		- 977.26		
$\Delta_f G^\circ =$		28.43		
$lnK_f =$		- 11.47		
Liquid ph	ase	014 (0		
$\Delta_{\mathbf{f}}H^{\circ} =$	204 (8	-311.62	0.60	200 4 D 444 17
$C_p^{\circ} =$	301.67	310.36	- 8.69	30PAR/HUF
S° =		414.94		
$\Delta_f S^\circ =$		- 1078.74		
$\Delta_f G^\circ =$		10.01		
$lnK_f =$		-4.04		

	Literatu	Reference		
Gas phase	•			
$\Delta_{\rm f}H^{\circ} =$	- 186.10	- 184.15	-1.95	47OSB/GIN
$C_p^{\circ} =$	141.88	142.34	-0.46	69STU/WES
<i>S</i> ° =	358.23	353.28	4.95	69STU/WES
$\Delta_f S^\circ =$		- 595.16		
$\Delta_f G^\circ =$		-6.70		
$lnK_f =$		2.70		
Liquid ph	ase			
$\Delta_{\mathbf{f}}H^{\circ} =$	-213.80	-211.35	-2.45	41PRO/ROS
$C_p^{\circ} =$	188.74	186.58	2.16	46DOU/HUF
S° =	272.00	266.93	5.07	46DOU/HUF
$\Delta_f S^\circ =$		- 681.51		
$\Delta_{f}G^{\circ} =$		-8.16		
$\ln K_{\rm f} =$		3.29		

(4×C-	2,2-Dimethylpentane $(4 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)_2) + (1 \times C - (C)_4) + (3 \times -CH_3 \text{ corr (quaternary)}), \sigma = 243$							
	Literatu	re – Calculated	= Residual	Reference				
Gas phase	;							
$\Delta_{\mathfrak{l}}H^{\circ} =$	-205.85	- 204.78	-1.07	47OSB/GIN				
$C_p^{\circ} =$	165.98	165.23	0.75	69STU/WES				
S° =	392.88	392.44	0.44	69STU/WES				
$\Delta_f S^\circ =$		-692.31						
$\Delta_f G^\circ =$		1.63						
$lnK_f =$		- 0.66						

TABLE 6. q-Alkanes (16) - Continued

TABLE 6. q-Alkanes (16) - Continued

	(C) + (2	\times C-(H) ₂ (C) ₂) ternary)), $\sigma =$		C ₇ H ₁₆		$H_{3}(C) + (3)$	$3 \times C$ -(H) ₂ (C) ₂) ternary)), $\sigma =$	1+ (1 × C-(C) ₄) - 81	C ₈ H ₁₈
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	i = Residual	Reference
Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se - 238.28 221.12 300.29	- 237.08 217.00 299.31 - 785.44 - 2.90 1.17	-1.20 4.12 0.98	41PRO/ROS2 61HUF/GRO 61HUF/GRO	Gas phase $\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$	-219.99 188.87 438.06	-220.85 188.12 440.73 -780.33 11.80 -4.76	0.86 0.75 - 2.67	47OSB/GIN 69STU/WES 69STU/WES
	H) ₃ (C)) + (3 corr (quat	\times C-(H) ₂ (C) ₂) ternary)), $\sigma =$ re – Calculated	243	C ₈ H ₁₈ + Reference	Liquid pha $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	- 257.53 246.60	-258.42 247.42 331.69 -889.37 6.75 -2.72	0.89 -0.82	45PRO/ROS 47OSB/GIN
Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$	-224.60 188.87 431.20	-225.41 188.12 431.60 -789.46	0.81 0.75 -0.40	47OSB/GIN 69STU/WES 69STU/WES		$H)_3(C)) + (1$	$\times C-(H)(C)_3)$ $(quat)), \sigma = 72$	+ (1 × C-(C) ₄) + 29	C7H16
$\Delta_t G^\circ = \ln K_t =$		9.97 -4.02				Literatu	re – Calculated	= Residual	Reference
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se - 261.88	- 262.81 247.42 331.69 - 889.37 2.36 - 0.95	0.93	45PRO/ROS	Gas phase $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	-204.47 164.56 383.60	- 202.27 165.26 378.70 - 706.04 8.24 - 3.32	- 2.20 - 0.70 4.90	47OSB/GIN 69STU/WES 69STU/WES
	H) ₃ (C)) + (2 ₃ corr (qua	×C-(H) ₂ (C) ₂) ternary)), $\sigma =$ re – Calculated	162	C ₇ H ₁₆ +	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se - 236.52 213.51 292.25	- 233.68 214.02 293.96 - 790.79 2.09 - 0.84	-2.84 -0.51 -1.71	41PRO/ROS2 61HUF/GRO 61HUF/GRO
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-201.17 165.98 399.70	-200.22 165.23 395.81 -688.94 5.19 -2.09	-0.95 0.75 3.89	47OSB/GIN 69STU/WES 69STU/WES	2,2,3-Trime (5×C-(H) ₃ (4×-CH	(C)) + (1×0) 3 corr (tert/ 0			C_8H_{18} + $(1 \times C - (C)_4)$ + Reference
Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se -234.18 214.80 305.60	-232.69 217.00 299.31 -785.44 1.49 -0.60	-1.49 -2.20 6.29	45PRO/ROS 76FIN/GRO 76FIN/GRO	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 219.99 188.87 425.18	-221.10 188.15 423.63 -797.43 16.65 -6.72	1.11 0.72 1.55	47OSB/GIN 69STU/WES 69STU/WES

TABLE 6. q-Alkanes (16) - Continued

TABLE 6. q-Alkanes (16) - Continued

2,2,3-Trimethylpentane (Continued)	C_8H_{18}	2,3,3-Trime	thylpentane	e (Continued)		C ₈ H ₁₈
$(5 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)_2) + (1 \times C - (H)(C)_2) + (1 \times C - (H)_3(C)_2) + (1 $	$)+(1\times C-(C)_4)+$			$C-(H)_2(C)_2)+(quat), \sigma = 24$		$(1 \times C - (C)_4) +$
Literature – Calculated = Residual	Reference		Literatu	re – Calculated :	= Residual	Reference
Liquid phase		Liquid pha	se			
$\Delta_t H^\circ = -256.90 -257.64 0.74$	45PRO/ROS	$\Delta_t H^\circ =$	-253.51	-257.64	4.13	45PRO/ROS
$C_p^{\circ} = 244.44$		$C_p^{\circ} =$	245.56	244.44	1.12	47OSB/GIN
$S^{\circ} = 326.34$		S° =		326.34		
$\Delta_t S^{\circ} = -894.72$		$\Delta_f S^\circ =$		-894.72		
$\Delta_{\rm f}G^{\circ} = 9.12$		$\Delta_{\rm f}G^{\circ} =$		9.12		
$\ln K_{\rm f} = -3.68$		$lnK_f =$		- 3.68		
2,2,4-Trimethylpentane	C ₈ H ₁₈		ramethylbut			C ₈ H ₁₈
(5 × C_(H)_(C)) ± (1 × C_(H)_(C)) ± (1 × C_(H)(C))+(1×C-(C))+			$\times C - (C)_4) +$	3122	
$(5 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)_2 + (1 \times C - (H)(C)_2)_2 + (1$	3) + (1 × C-(C)4) +	(ox-CH		$t/quat$)), $\sigma = 1$		
Literature – Calculated = Residual	Reference		Literatur	re – Calculated =	= Residual	Reference
		Gas phase				
Gas phase		$\Delta_t H^{\circ} =$	-225.22	-219.00	-6.22	47OSB/GIN
$\Delta_t H^{\circ} = -224.01 -222.90 -1.11$	47OSB/GIN	$C_n^{\circ} =$	192.59	187.44	5.15	69STU/WES
$C_p^{\circ} = 188.87 188.15 0.72$	69STU/WES	S° =	389.36	386.10	3.26	69STU/WES
$S^{\circ} = 423.21 417.86 5.35$	69STU/WES	Δ _ι S° =		-834.96		
$\Delta_t S^{\circ} = -803.20$		$\Delta_{\rm f}G^{\circ} =$		29.94		
$\Delta_{\rm f}G^{\circ} = 16.57$		$lnK_f =$		-12.08		
$\ln K_{\rm f} = -6.69$		<u> </u>				
** • • •		Liquid pha	se	252.52		
Liquid phase	45DD O/D O/I	$\Delta_{\mathbf{f}}H^{\circ} =$		-253.52		
$\Delta_t H^\circ = -259.16 -259.41 0.25$	45PRO/ROS	$C_p^{\circ} = S^{\circ} =$		239.36		
$C_p^{\circ} = 238.57$ 244.44 -5.87 $S^{\circ} = 328.03$ 326.34 1.69	47OSB/GIN 40PIT	$\Delta_{\mathbf{f}}S^{\circ} =$		302.50 - 918.56		
$\Delta_{t}S^{\circ} = 528.03 520.34 1.09$ $\Delta_{t}S^{\circ} = -894.72$	40F11	$\Delta_i G^\circ =$		20.35		
$\Delta_t G^{\circ} = 7.35$		$\ln K_{\ell} =$		-8.21		
$\ln K_{\rm f} = -2.97$					•,	
		Solid phase		•		
2.2.2.75-1	O 11	$\Delta_{i}H^{\circ} =$	- 268.61	- 268.94	0.33	45PRO/ROS
2,3,3-Trimethylpentane	C_8H_{18}	$C_p^{\circ} =$	237.44	237.44	0.00	52SCO/DOU
(5 × C_(U)_(C)) ± (1 × C_(U)_(C) \ + (1 × C_(U)(C))+(1×C-(C))+	$S^{\circ} = \Delta_{f}S^{\circ} =$	273.76	273.76 947.30	0.00	52SCO/DOU
$(5 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)_3(C)_3 + (1 \times C - (H)(C)_3(C)_3) + (1 \times C - (H)(C)_3(C)_3(C)_3 + (1 \times C - (H)(C)_3(C)_3) + (1 \times C - (H)(C)_3(C)_3(C)_3 + (1 \times C - (H)(C)_3(C)_3) + (1 \times C - (H)(C)_3(C)_3(C)_3 + (1 \times C - (H)(C)_3(C)_3) + (1 \times C - (H)(C)_3(C)_3(C)_3 + (1 \times C - (H)(C)_3(C)_3) + (1 \times C - (H)(C)_3(C)_3(C)_3 + (1 \times C - (H)(C)_3(C)_3) + (1 \times C - (H)(C)_3(C)_3(C)_3(C)_3(C)_3(C)_3(C)_3(C)_$	3)+(1×U-(U)4)+	$\Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} =$		- 947.30		
$(4 \times -CH_3 \text{ corr } (tert/quat)), \sigma = 243$		$\Delta_t G^{\circ} = \ln K_t =$		13.50 5.44		
Literature – Calculated = Residual	Reference					
Gas phase			amethylpen			C ₉ H ₂₀
$\Delta_i H^{\circ} = -216.27 -221.10$ 4.83	47OSB/GIN			\times C-(H) ₂ (C) ₂) +		+
$C_{\mu}^{\circ} - 188.87 188.15 0.72$	69STU/WES	(5 × -CH	3 corr (quat	$(quat)$, $\sigma = 2$	10/	
$S^{\circ} = 431.54 427.00 4.54$	69STU/WES		Litonot	e – Calculated =	- Desidual	Reference
$\Delta_t S^{\circ} = -794.06$			Literatur	e – Calculated =	- Vesignai	Reference
$\Delta_t G^{\circ} = 15.65$			····			
$\ln K_{\rm f} = -6.31$		Gas phase				
		$\Delta_f H^\circ =$	-237.11	-238.99	1.88	61LAB/GRE
				A	1.00	
				210.33	1.76	69STU/WES
		$C_p^{\circ} = S^{\circ} =$	212.09 446.39	210.33 440.16	1.76 6.23	69STU/WES 69STU/WES
		$C_p^{\circ} =$	212.09	210.33 440.16 -917.21		69STU/WES 69STU/WES
		$C_p^{\circ} = S^{\circ} =$	212.09	440.16		

TABLE 6. q-Alkanes (16) - Continued

TABLE 6. q-Alkanes (16) - Continued

(6×C-(I	$H_{3}(C)) + (1$	tane (Continue \times C-(H) ₂ (C) ₂)/quat)), $\sigma = 2$	$+(2\times C-(C)_4)$	C ₉ H ₂₀	(4×C-(1		ne $S \times C - (H)_2(C)_2$ ternary)), $\sigma =$		C ₈ H ₁	
	Literatur	e – Calculated	= Residual	Reference	Literature - Calculated = Residual			= Residual	Reference	
Liquid pha	se				Gas phase					
$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} =$	-278.28	-278.61 269.78 334.88 -1022.49 26.25 -10.59	0.33	47JOH/PRO	$\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$	-214.85 188.87 432.96	-216.29 188.12 431.60 -789.46 19.09 -7.70	1.44 0.75 1.36	47OSB/GIN 69STU/WES 69STU/WES	
					Liquid pha	se				
(6×C-(1	2,2,4,4-Tetramethylpentane $(6 \times C-(H)_3(C)) + (1 \times C-(H)_2(C)_2) + (2 \times C-(C)_4) + (6 \times -CH_3 \text{ corr } (quat/quat)), \sigma = 13122$ Literature – Calculated = Residual			C ₉ H ₂₀	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = 0$	- 252.84	-254.03 247.42 331.69 -889.37 11.14	1.19	45PRO/ROS	
							-4.49			
Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	-241.84 211.63 431.50	-239.63 210.33 425.26 -932.11 38.28	-2.21 1.30 6.24	61LAB/GRE 69STU/WES 69STU/WES	3,3-Diethyl (4 × C-(I	H)3(C))+(4	\times C-(H) ₂ (C) ₂) re – Calculated		C_9H_{24}), $\sigma = 972$ Reference	
$lnK_f =$		- 15.44		<u></u>						
Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	se - 279.99	- 279.25 269.78 334.88 - 1022.49 25.61 - 10.33	- 0.74	47JOH/PRO	Gas phase $\Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$	- 232.34 204.18 461.54	- 232.36 211.01 459.23 - 898.14 35.42 - 14.29	0.02 - 6.83 2.31	61LAB/GRE 69STU/WES 69STU/WES	
(7×C-(1	l ₃ corr (quat			C ₁₀ H ₂₂	Liquid phat $ \Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = $	se -275.39 278.80 333.40	-275.37 277.84 364.07 -993.30 20.78 -8.38	0.02 0.96 30.67	47JOH/PRO 76FIN/MES 76FIN/MES	
									·····	
Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_f =$	234.43 462.83	-263.07 233.25 456.45 -1037.23 46.18 -18.63	1.18 6.38	69STU/WES 69STU/WES						
Liquid pha $\Delta_i H^\circ = C_p^\circ =$	se	-306.54 297.22								
$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f =$		361.91 -1131.77 30.90 -12.46								

TABLE 7. n-Alkenes (32)

89.30

-36.02

 $lnK_f =$

Ethylene (2×C _d (F	$H)_2), \sigma = 4$			C ₂ H ₄		$(1)_3(C) + (1)_3(C)$	\times C-(H) ₂ (C) ₂) \times C _d -(H) ₂), σ		$(C)(C_d)$ +
	Literature	- Calculated	= Residual	Reference	, ,	Literatur	re – Calculated	= Residual	Reference
Gas phase					. , 				
$\Delta_i H^{\circ} =$	52.50	52.64	-0.14	37ROS/KNO	Liquid phas	se			
$C_P^{\circ} =$	42.84	42.76	0.08	75CHA/ZWO	$\Delta_{\rm f}H^{\circ} =$	- 46.97	- 46.27	-0.70	79GOO/SMI
S° =	219.20	219.51	-0.31	75CHA/ZWO	$C_{\rho}^{\circ} =$	154.87	149.16	5.71	90MES/TOD
$\Delta_{\mathbf{f}}S^{\circ} =$		-53.11			S° =	262.60	262.12	0.48	90MES/TOD
$\Delta_{\rm f}G^{\circ} =$		68.47			$\Delta_f S^\circ =$		-419.43		
$lnK_f =$		-27.62			$\Delta_f G^\circ =$		78.78		
					$lnK_f =$		-31.78		
Propylene				C₃H ₆					
	I) ₃ (C))+(1	$\times C_{d}$ - $(H)_2)+(1$	$1 \times C_d$ – $(H)(C)$		1-Hexene				C₅H₁
	Literatur	e – Calculated	= Residual	Reference			\times C-(H) ₂ (C) ₂) C _d -(H)(C)), σ		(C)(C _d))+
Gas phase						Literatur	re – Calculated	= Residual	Reference
$\Delta_i H^\circ =$	19.76	20.38	-0.62	37ROS/KNO		· , , · · · · · · · · · · · · · · · · ·			
$C_p^{\circ} =$	64.31	65.85	- 1.54	75CHA/ZWO	Gas phase				
S° =	266.60	266.76	-0.16	75CHA/ZWO	$\Delta_t H^\circ =$	-41.51	-41.76	0.25	56CAM/ROS
$\Delta_t S^\circ =$	200.00	-142.18	-0.10	BOILDENO	$C_p^{\circ} =$	132.34	132.26	0.23	69STU/WES
$\Delta_{\mathbf{f}}G^{\circ} =$		62.77			$S^{\circ} =$	384.64	383.28	1.36	69STU/WES
$lnK_f =$		-25.32			$\Delta_{f}S^{\circ} =$	304.04	- 434.59	1.50	0931 U/WE3
		20.02					87.81		
-					A430 =				
		·	.,		$\Delta_f G^\circ = \ln K_f =$		-35.42		
1-Butene				C ₄ H ₈					
1-Butene	I)₃(C))+(1:	× C _d (H) ₂) + (1×C _d −(H)(C)			se			
1-Butene (1×C-(H	I) ₃ (C))+(1: I) ₂ (C)(C _d)),		1×C _d −(H)(C)		$lnK_f =$ Liquid phas $\Delta_t H^\circ =$	se -72.22		-0.22	59SKE/SNE
1-Butene (1×C-(H			1×C _d −(H)(C)		$lnK_f =$ Liquid phas		-35.42	-0.22 3.72	59SKE/SNE 57MCC/FIN2
1-Butene (1×C-(H	I) ₂ (C)(C _d)),				$lnK_f =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$	-72.22	-35.42 -72.00		
1-Butene (1×C-(H	I) ₂ (C)(C _d)),	$\sigma = 3$)+	$\ln K_{\rm f} = \frac{1}{1}$ Liquid phas $\Delta_{\rm f} H^{\circ} = C_{\rm p}^{\circ} = \frac{1}{1}$	-72.22 183.30	-35.42 -72.00 179.58	3.72	57MCC/FIN2
1-Butene (1×C-(H	I) ₂ (C)(C _d)),	$\sigma = 3$)+	$lnK_f =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$	-72.22 183.30	-72.00 179.58 294.50	3.72	57MCC/FIN2
1-Butene (1×C-(F (1×C-(F	I) ₂ (C)(C _d)),	$\sigma = 3$	= Residual)+		-72.22 183.30	-35.42 -72.00 179.58 294.50 -523.37	3.72	57MCC/FIN2
1-Butene $(1 \times C - (H + (1 \times C - (H + (1 \times C + (H + (1 \times C + (H + $	$I)_2(C)(C_d)$, Literatur -0.54	$\sigma = 3$)+	$ \begin{array}{c} lnK_f = \\ \hline Liquid phas \\ \Delta_t H^\circ = \\ C_p^\circ = \\ S^\circ = \\ \Delta_t S^\circ = \\ \Delta_t G^\circ = \\ \end{array} $	-72.22 183.30	-72.00 179.58 294.50 -523.37 84.04	3.72	57MCC/FIN2
1-Butene (1×C-(H (1×C-(H	I) ₂ (C)(C _d)), Literatur	σ = 3 e – Calculated	= Residual	Reference	$ \begin{array}{c} lnK_f = \\ \hline Liquid phas \\ \Delta_t H^\circ = \\ C_p^\circ = \\ S^\circ = \\ \Delta_t S^\circ = \\ \Delta_t G^\circ = \\ \end{array} $	-72.22 183.30	-72.00 179.58 294.50 -523.37 84.04	3.72	57MCC/FIN2
1-Butene $(1 \times C - (F + (1 \times C $	$I)_2(C)(C_d)$, Literatur -0.54	σ = 3 e – Calculated -0.50	= Residual - 0.04	Reference 51PRO/MAR	$ \begin{array}{c} lnK_f = \\ \hline Liquid phas \\ \Delta_t H^\circ = \\ C_p^\circ = \\ S^\circ = \\ \Delta_t S^\circ = \\ \Delta_t G^\circ = \\ \end{array} $	-72.22 183.30	-72.00 179.58 294.50 -523.37 84.04	3.72	57MCC/FIN2
1-Butene $(1 \times C - (F + (1 \times C + (1 \times C - (F + (1 \times C)))))))))))))))))$ Gas phase Δ_{i} C_{i} $C_$	I) ₂ (C)(C _d)), Literatur - 0.54 85.65	σ = 3 e - Calculated -0.50 86.48	= Residual - 0.04 - 0.83	Reference 51PRO/MAR 69STU/WES	$\ln K_f = \frac{1}{\text{Liquid phas}}$ $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \frac{1}{\text{ln} K_f} = \frac{1}{\text{-Heptene}}$	-72.22 183.30 295.18	-72.00 179.58 294.50 -523.37 84.04 -33.90	3.72 0.68	57MCC/FIN2 57MCC/FIN2 C ₂ H ₁₄
1-Butene $(1 \times C - (F + G))$ $(1 \times C - (F + G))$ Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = S^{\circ} = S^{\circ}$	I) ₂ (C)(C _d)), Literatur - 0.54 85.65	σ = 3 e - Calculated -0.50 86.48 304.96 -240.29 71.14	= Residual - 0.04 - 0.83	Reference 51PRO/MAR 69STU/WES	In $K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_f^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\ln K_f =$ 1-Heptene $(1 \times C - (H^\circ)^{-1})^{-1}$	-72.22 183.30 295.18	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂)	3.72 0.68 + (1 × C-(H) ₂ (57MCC/FIN2 57MCC/FIN2 C ₂ H ₁₄
1-Butene $(1 \times C - (F + (1 \times C + (1 \times C - (F + (1 \times C)))))))))))))))))$ Gas phase Δ_{i} C_{i} $C_$	I) ₂ (C)(C _d)), Literatur - 0.54 85.65	σ = 3 e - Calculated -0.50 86.48 304.96 -240.29	= Residual - 0.04 - 0.83	Reference 51PRO/MAR 69STU/WES	In $K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_f^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\ln K_f =$ 1-Heptene $(1 \times C - (H^\circ)^{-1})^{-1}$	-72.22 183.30 295.18	-72.00 179.58 294.50 -523.37 84.04 -33.90	3.72 0.68 + (1 × C-(H) ₂ (57MCC/FIN2 57MCC/FIN2 C-H14
1-Butene $(1 \times C - (F + G))$ $(1 \times C - (F + G))$ Gas phase $\Delta_{\mu}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{\rho}S^{\circ} = \Delta_{\rho}G^{\circ} = S^{\circ} = S^{\circ}$	I) ₂ (C)(C _d)), Literatur - 0.54 85.65	σ = 3 e - Calculated -0.50 86.48 304.96 -240.29 71.14	= Residual - 0.04 - 0.83	Reference 51PRO/MAR 69STU/WES	In $K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_f^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\ln K_f =$ 1-Heptene $(1 \times C - (H^\circ)^{-1})^{-1}$	-72.22 183.30 295.18 I) ₃ (C))+(3 H) ₂)+(1×0	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂)	$3.72 \\ 0.68$ $+ (1 \times C - (H)_{2}(H)$	57MCC/FIN2 57MCC/FIN2 C-H14
1-Butene $(1 \times C - (H + 1) \times$	-0.54 85.65 305.60	σ = 3 e - Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70	= Residual - 0.04 - 0.83 0.64	Reference 51PRO/MAR 69STU/WES 69STU/WES	$lnK_f =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $lnK_t =$ 1-Heptene $(1 \times C_t - (1 \times C_t))$	-72.22 183.30 295.18 I) ₃ (C))+(3 H) ₂)+(1×0	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) -C _d -(H)(C)), σ	$3.72 \\ 0.68$ $+ (1 \times C - (H)_{2}(H)$	57MCC/FIN2 57MCC/FIN2 C ₇ H ₁₄ (C)(C _d)) +
1-Butene $(1 \times C - (H + 1) \times$	-0.54 85.65 305.60	σ = 3 e – Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70 × C-(H) ₂ (C) ₂)	= Residual - 0.04 - 0.83 0.64 + (1 × C-(H) ₂	Reference 51PRO/MAR 69STU/WES 69STU/WES	$lnK_{f} = \frac{1}{Liquid phas}$ $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = lnK_{f} = \frac{1}{Light}$ $1-Heptene (1 \times C_{-}(Hight))$ $(1 \times C_{d}^{-}(Hight))$ $Gas phase$	-72.22 183.30 295.18 I) ₃ (C))+(3 H) ₂)+(1×0 Literatur	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) C _d -(H)(C)), σ re - Calculated	3.72 0.68 + (1 × C-(H) ₂ (= 3 = Residual	57MCC/FIN2 57MCC/FIN2 C ₂ H ₁₋₄ (C)(C _d)) +
1-Butene $(1 \times C - (H + 1) \times$	-0.54 85.65 305.60	σ = 3 e - Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70	= Residual - 0.04 - 0.83 0.64 + (1 × C-(H) ₂	Reference 51PRO/MAR 69STU/WES 69STU/WES	In $K_f =$ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ 1-Heptene $(1 \times C - (H \times C_d - (I \times C_d + H)))$ Gas phase $\Delta_t H^\circ = I = I = I = I = I$	-72.22 183.30 295.18 I) ₃ (C)) + (3 H) ₂) + (1 × 0 Literatur -62.72	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) -C _d -(H)(C)), σ	$3.72 \\ 0.68$ $+ (1 \times C - (H)_{2}(H)$	57MCC/FIN2 57MCC/FIN2 C ₂ H ₁₋₄ (C)(C _d)) +
1-Butene $(1 \times C - (H + 1) \times$	-0.54 85.65 305.60	σ = 3 e – Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70 × C-(H) ₂ (C) ₂) × C _a -(H) ₂), σ	= Residual -0.04 -0.83 0.64 + (1 × C-(H) ₂ = 3	Reference 51PRO/MAR 69STU/WES 69STU/WES C5H10 (C)(Cd))+	In $K_f =$ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ 1-Heptene (1 × C-(H) (1 × C_d-(I) Gas phase $\Delta_t H^\circ = C_p^\circ =$	-72.22 183.30 295.18 I) ₃ (C))+(3 H) ₂)+(1×0 Literatur -62.72 155.23	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) C _d -(H)(C)), σ re - Calculated	3.72 0.68 + (1 × C-(H) ₂ (= 3 = Residual -0.33 0.08	57MCC/FIN2 57MCC/FIN2 C ₇ H ₁₄ (C)(C _d)) +
1-Butene $(1 \times C - (H + 1) \times$	-0.54 85.65 305.60	σ = 3 e – Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70 × C-(H) ₂ (C) ₂)	= Residual -0.04 -0.83 0.64 + (1 × C-(H) ₂ = 3	Reference 51PRO/MAR 69STU/WES 69STU/WES	In $K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ In $K_t =$ 1-Heptene (1 × C-(H) (1 × C _d -(I) Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$	-72.22 183.30 295.18 I) ₃ (C)) + (3 H) ₂) + (1 × 0 Literatur -62.72	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) C _d -(H)(C)), σ e - Calculated -62.39 155.15 422.44	3.72 0.68 $+ (1 \times C - (H)_{2})$ = Residual - 0.33	57MCC/FIN2 57MCC/FIN2 C ₇ H ₁₄ (C)(C _d)) + Reference
1-Butene $(1 \times C - (H + 1) \times$	-0.54 85.65 305.60	σ = 3 e – Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70 × C-(H) ₂ (C) ₂) × C _a -(H) ₂), $σ$	= Residual -0.04 -0.83 0.64 + (1 × C-(H) ₂ = 3	Reference 51PRO/MAR 69STU/WES 69STU/WES C5H10 (C)(Cd))+	In $K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ In $K_f =$ 1-Heptene (1 × C-(F) (1 × C _d -(I) Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$	-72.22 183.30 295.18 I) ₃ (C))+(3 H) ₂)+(1×0 Literatur -62.72 155.23	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) -C _d -(H)(C)), σ re - Calculated -62.39 155.15	3.72 0.68 + (1 × C-(H) ₂ (= 3 = Residual -0.33 0.08	57MCC/FIN2 57MCC/FIN2 C ₇ H ₁₄ (C)(C _d)) + Reference 50FOR/CAM 69STU/WES
1-Butene $(1 \times C - (H + G))$ $(1 \times C - (H + G))$ Gas phase $\Delta_t H^o = C_p^o = S^o = \Delta_t S^o = \Delta_t S^o = \Delta_t S^o = \Lambda_t S^o = \Lambda$	-0.54 85.65 305.60	σ = 3 e – Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70 × C-(H) ₂ (C) ₂) × C _a -(H) ₂), $σ$	= Residual -0.04 -0.83 0.64 + (1 × C-(H) ₂ = 3	Reference 51PRO/MAR 69STU/WES 69STU/WES C5H10 (C)(Cd))+	In $K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ In $K_f =$ 1-Heptene $(1 \times C_d - (1 \times $	-72.22 183.30 295.18 I) ₃ (C))+(3 H) ₂)+(1×0 Literatur -62.72 155.23	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) C _d -(H)(C)), σ e - Calculated -62.39 155.15 422.44	3.72 0.68 + (1 × C-(H) ₂ (= 3 = Residual -0.33 0.08	57MCC/FIN2 57MCC/FIN2 C ₇ H ₁₄ (C)(C _d)) + Reference 50FOR/CAM 69STU/WES
1-Butene $(1 \times C - (H + 1) \times $	-0.54 85.65 305.60 H) ₃ (C)) + (1 H)(C)) + (1 Literatur	σ = 3 e - Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70 × C-(H) ₂ (C) ₂) × C _σ -(H) ₂), σ e - Calculated	= Residual -0.04 -0.83 0.64 + (1 × C-(H) ₂ = 3 = Residual	Reference 51PRO/MAR 69STU/WES 69STU/WES C ₅ H ₁₀ (C)(C _d))+ Reference	In $K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ In $K_f =$ 1-Heptene (1 × C-(F) (1 × C _d -(I) Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$	-72.22 183.30 295.18 I) ₃ (C))+(3 H) ₂)+(1×0 Literatur -62.72 155.23	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) -C _d -(H)(C)), σ re - Calculated -62.39 155.15 422.44 -531.74	3.72 0.68 + (1 × C-(H) ₂ (= 3 = Residual -0.33 0.08	57MCC/FIN2 57MCC/FIN2 C ₇ H ₁₄ (C)(C _d)) + Reference 50FOR/CAM 69STU/WES
1-Butene $(1 \times C - (H + I) \times $	-0.54 85.65 305.60 H) ₃ (C)) + (1 Literatur	σ = 3 e – Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70 × C-(H) ₂ (C) ₂) × C _a -(H) ₂), $σ$	= Residual -0.04 -0.83 0.64 + (1 × C-(H) ₂ = 3	Reference 51PRO/MAR 69STU/WES 69STU/WES C5H10 (C)(Cd))+	In $K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ In $K_f =$ 1-Heptene $(1 \times C_d - (1 \times $	-72.22 183.30 295.18 I) ₃ (C))+(3 H) ₂)+(1×0 Literatur -62.72 155.23	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) -C _d -(H)(C)), σ re - Calculated -62.39 155.15 422.44 -531.74 96.15	3.72 0.68 + (1 × C-(H) ₂ (= 3 = Residual -0.33 0.08	57MCC/FIN2 57MCC/FIN2 C ₂ H ₁ . (C)(C _d)) + Reference 50FOR/CAM 69STU/WES
1-Butene $(1 \times C - (H + C))))))))))))$ Gas phase $C_{\mu}^{\mu} = C_{\mu}^{\mu} = C_{\mu}^{\mu} = C_{\mu}^{\mu} = C_{\mu}^{\mu} = C_{\mu}^{\mu} = C_{\mu}^{\mu} = C_{\mu}^{\mu})$	-0.54 85.65 305.60 H) ₃ (C)) + (1 H)(C)) + (1 Literatur	σ = 3 e - Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70 × C-(H) ₂ (C) ₂) × C _σ -(H) ₂), σ e - Calculated	= Residual -0.04 -0.83 0.64 + (1 × C-(H) ₂ = 3 = Residual	Reference 51PRO/MAR 69STU/WES 69STU/WES C ₅ H ₁₀ (C)(C _d))+ Reference	In $K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ In $K_f =$ 1-Heptene $(1 \times C_d - (1 \times $	-72.22 183.30 295.18 I) ₃ (C))+(3 H) ₂)+(1×0 Literatur -62.72 155.23	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) -C _d -(H)(C)), σ re - Calculated -62.39 155.15 422.44 -531.74 96.15	3.72 0.68 + (1 × C-(H) ₂ (= 3 = Residual -0.33 0.08	57MCC/FIN2 57MCC/FIN2 C ₂ H ₁ . (C)(C _d)) + Reference 50FOR/CAM 69STU/WES
1-Butene $(1 \times C - (H + I) \times $	-0.54 85.65 305.60 H) ₃ (C)) + (1 Literatur	σ = 3 e - Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70 × C-(H) ₂ (C) ₂) × C _σ -(H) ₂), σ e - Calculated	= Residual -0.04 -0.83 0.64 + (1 × C-(H) ₂ = 3 = Residual	Reference 51PRO/MAR 69STU/WES 69STU/WES C ₅ H ₁₀ (C)(C _d))+ Reference	In $K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ In $K_f =$ 1-Heptene $(1 \times C_d - (1 \times $	-72.22 183.30 295.18 I) ₃ (C)) + (3 H) ₂) + (1 × 0 Literatur -62.72 155.23 423.59	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) -C _d -(H)(C)), σ re - Calculated -62.39 155.15 422.44 -531.74 96.15	3.72 0.68 + (1 × C-(H) ₂ (= 3 = Residual -0.33 0.08	57MCC/FIN2 57MCC/FIN2 C ₂ H ₁ . (C)(C _d)) + Reference 50FOR/CAM 69STU/WES
1-Butene $(1 \times C - (H + I) \times $	-0.54 85.65 305.60 H) ₃ (C)) + (1 Literatur -21.50 109.58	σ = 3 e - Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70 × C-(H) ₂ (C) ₂) × C _a -(H) ₂ , σ e - Calculated -21.13 109.37	= Residual -0.04 -0.83 0.64 + (1 × C-(H) ₂ = 3 = Residual -0.37 0.21	Reference 51PRO/MAR 69STU/WES 69STU/WES C ₅ H ₁₀ (C)(C _d))+ Reference 86TRC 69STU/WES	In $K_f =$ Liquid phas $\Delta_t H^\circ =$ $C^\circ_p =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ In $K_t =$ 1-Heptene $(1 \times C - (H + 1) \times C_{\sigma} - (H +$	-72.22 183.30 295.18 I) ₃ (C)) + (3 H) ₂) + (1 × 0 Literatur -62.72 155.23 423.59	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) -C _d -(H)(C)), σ re - Calculated -62.39 155.15 422.44 -531.74 96.15	3.72 0.68 + (1 × C-(H) ₂ (= 3 = Residual -0.33 0.08	57MCC/FIN2 57MCC/FIN2 C ₂ H ₄ (C)(C _d)) + Reference 50FOR/CAM 69STU/WES
1-Butene $(1 \times C - (H + I) \times $	-0.54 85.65 305.60 H) ₃ (C)) + (1 Literatur -21.50 109.58	σ = 3 e – Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70 $× C-(H)2(C)2) × Ca-(H)2, σ e – Calculated -21.13 109.37 344.12 -337.44$	= Residual -0.04 -0.83 0.64 + (1 × C-(H) ₂ = 3 = Residual -0.37 0.21	Reference 51PRO/MAR 69STU/WES 69STU/WES C ₅ H ₁₀ (C)(C _d))+ Reference 86TRC 69STU/WES	In $K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ In $K_t =$ 1-Heptene (1 × C-(H) (1 × C _d -(I) Gas phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ In $K_t =$ Liquid phas $\Delta_t H^\circ =$	-72.22 183.30 295.18 I) ₃ (C)) + (3 H) ₂) + (1 × 0 Literatur -62.72 155.23 423.59	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) C _d -(H)(C)), σ re - Calculated = -62.39 155.15 422.44 -531.74 96.15 -38.79	3.72 0.68 + (1×C-(H) ₂ (= 3 = Residual -0.33 0.08 1.15	57MCC/FIN2 57MCC/FIN2 C ₂ H ₄ (C)(C _d)) + Reference 50FOR/CAM 69STU/WES 69STU/WES
1-Butene $(1 \times C - (H + I) \times $	-0.54 85.65 305.60 H) ₃ (C)) + (1 Literatur -21.50 109.58	σ = 3 e – Calculated -0.50 86.48 304.96 -240.29 71.14 -28.70 $× C-(H)2(C)2) × Ca-(H)2, σ e – Calculated -21.13 109.37 344.12$	= Residual -0.04 -0.83 0.64 + (1 × C-(H) ₂ = 3 = Residual -0.37 0.21	Reference 51PRO/MAR 69STU/WES 69STU/WES C ₅ H ₁₀ (C)(C _d))+ Reference 86TRC 69STU/WES	In $K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ In $K_t =$ 1-Heptene $(1 \times C - (H + 1) \times C_d - (H + 1) \times C_d - (H + 1)$ Gas phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ In $K_t =$ Liquid phas	-72.22 183.30 295.18 I) ₃ (C)) + (3 H) ₂) + (1 × 0 Literatur -62.72 155.23 423.59	-35.42 -72.00 179.58 294.50 -523.37 84.04 -33.90 × C-(H) ₂ (C) ₂) C _d -(H)(C)), σ re - Calculated = -62.39 155.15 422.44 -531.74 96.15 -38.79	3.72 0.68 + (1 × C-(H) ₂ (= 3 = Residual -0.33 0.08 1.15	57MCC/FIN2 57MCC/FIN2 C ₂ H ₄ (C)(C _d)) + Reference 50FOR/CAM 69STU/WES 69STU/WES

TABLE 7. q-Alkanes (16) - Continued

TABLE 7. q-Alkanes (16) - Continued

		× C-(H) ₂ (C) ₂) C _d -(H)(C)), σ		$(C)(C_d)) +$	(1×C-((Continued) H) ₃ (C)) + (6 (H)(C)) + (1	$6 \times C$ - $(H)_2(C)_2$ $6 \times C_d$ - $(H)_2$), σ	$\begin{array}{l} + (1 \times C - (H)) \\ = 3 \end{array}$	$C_{10}H_{20}$ $C(C)(C_d)) +$
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	l = Residual	Reference
Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 82.93 178.07 462.54	-83.02 178.04 461.60 -628.89 104.48 -42.15	0.09 0.03 0.94	50FOR/CAM 69STU/WES 69STU/WES	Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f =$	- 173.80 300.83 425.01	-174.92 301.26 424.02 -939.09 105.07 -42.38	1.12 - 0.43 0.99	61ROC/ROS 57MCC/FIN2 57MCC/FIN2
Liquid phas $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S$	se - 123.80 241.21 360.45	- 123.46 240.42 359.26 - 731.23 94.56	-0.34 0.79 1.19	61ROC/ROS 57MCC/FIN2 57MCC/FIN2		H) ₃ (C))+(1 (H)(C))+(1	$2 \times C - (H)_2(C)_2 \times C_d - (H)_2), \sigma$ re – Calculated	= 3	$C_{16}H_{32}$ $C_{16}C_{10}C$
	H)(C))+(1	-38.14 $\times C-(H)_2(C)_2$ $\times C_d-(H)_2), \sigma$ The - Calculated	= 3	C_9H_{18} $(C)(C_d)) +$ Reference	Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t =$	- 249.16 361.04 774.12	-248.06 361.16 774.88 -1406.10 171.17 -69.05	- 1.10 - 0.12 - 0.76	70ZWO/WIL 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \ln K_t = \Delta_t S^\circ = \Delta_t $	-103.51 200.96 501.49	103.65 200.93 500.76 726.04 112.82 45.51	0.14 0.03 0.73	69STU/WES 69STU/WES 69STU/WES	Liquid pha $\Delta_{\mathbf{f}}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{\mathbf{f}}S^{\circ} = \Delta_{\mathbf{f}}G^{\circ} = \ln K_{\mathbf{f}} = 0$	se - 329.24 483.34 613.88	- 329.30 483.78 618.30 - 1562.68 136.61 - 55.11	0.06 0.44 4.42	55FRA/PRO 90MES/TOD 90MES/TOD
$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = 0$	se 149.03 270.36 392.54	149.19 270.84 391.64 835.16 99.81	0.16 -0.48 0.90	86TRC 90MES/TOD 90MES/TOD		H) ₃ (C)) + (2 insat) corr),	$ \times C_{d} - (H)(C)) - $ $ \sigma = 18 $ $ e - Calculated $		C ₄ H ₈
	H)(C))+(1	-40.26 $\times \text{C(H)}_2(\text{C)}_2)$ $\times \text{C}_{\sigma}(\text{H)}_2), \sigma$ The - Calculated	= 3	$C_{10}H_{20}$ $(C)(C_d))+$ Reference	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = $	-7.57 78.91 300.83	-7.03 80.91 301.77 -243.48 65.56 -26.45	- 0.54 - 2.00 - 0.94	51PRO/MAR 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_f =$	-123.34 223.80 540.45	-124.28 223.82 539.92 -823.19 121.16 -48.87	0.94 -0.02 0.53	50FOR/CAM 69STU/WES 69STU/WES					

TABLE 7.	n-Alkenes	(32) -	Continued
IADLE /.	W-WRCHC2	1321 -	Commuca

TARIE	7	n-Alkenes	(32)	Continued
IADLE		" -VINCHES	1321 -	Commucu

	ene {}) ₃ (C)) + (2)	< C _d −(H)(C)),	$\sigma = 18$	C_4H_8	cis-2-Hexen (2×C-(H		× C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂	C ₆ H (C)(C ₄))+
	-/3(-// (-	-4 ()(-)//					× cis (unsat) co		(-/(-6//
	Literatur	e – Calculated :	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase						· · · · · · · · · · · · · · · · · · ·			
$\Delta_{\mathbf{f}}H^{\circ} = 0$	-10.97	-11.88	0.91	51PRO/MAR	Gas phase				
$C_p^{\circ} =$	87.82	88.94	-1.12	69STU/WES	$\Delta_t H^{\circ} =$	-52.34	-48.54	-3.80	56CAM/ROS
S° =	296.48	296.71	-0.23	69STU/WES	$C_p^{\circ} =$	125.69	124.43	1.26	69STU/WES
$\Delta_f S^\circ =$		-248.54			S° =	386.48	384.89	1.59	69STU/WES
$\Delta_{\mathbf{f}}G^{\circ} =$		62.22			$\Delta_{\rm f} S^{\circ} =$		- 432.97		
$lnK_f =$		-25.10			$\Delta_t G^{\circ} =$		80.55		
					$lnK_f =$		- 32.49 		
cis -2-Penter	ne			C ₅ H ₁₀	Liquid phas	se			
(2×C-(F	$H_{3}(C) + (1)$	× C-(H) ₂ (C)(C	(a)) + $(2 \times C_{a}$		$\Delta_{\mathbf{f}}H^{\circ} =$	-83.89	-79.31	-4.58	60BAR/ROS
	insat) corr),				$C_p^{\circ} =$	178.36	181.87	-3.51	90MES/TOD
•					S° =	291.86	287.81	4.05	90MES/TOD
	Literatur	e – Calculated	= Residual	Reference	$\Delta_{\mathbf{f}}S^{\circ} =$		-530.06		
		<u> </u>			$\Delta_{\mathbf{f}}G^{\circ} =$		78.73		
Gas phase					$lnK_f =$		-31.76		
$\Delta_t H^\circ =$	-26.67	-27.91	1.24	86TRC		 -			
$C_p^{\circ} =$	101.75	101.54	0.21	69STU/WES					
S° =	346.27	345.73	0.54	69STU/WES	trans -2-Hex				C ₆ H
$\Delta_f S^\circ =$		-335.82			(2×C-(F	$I_{3}(C) + (1$	\times C-(H) ₂ (C) ₂)	$+(1\times C-(H)_2)$	$(C)(C_d)$ +
$\Delta_f G^\circ =$		72.22			$(2 \times C_d - (1))$	$H)(C)), \sigma =$	= 9		
$lnK_f =$		-29.13				Literatur	e – Calculated	- Desidual	Deference
	· ·	 				Literatur		- Residuai	Reference
Liquid phas $\Delta_t H^\circ =$		_ 52 50	0.00	70G00/8MI	Goo -bo				
•	53.49	-53.58	0.09	79GOO/SMI	Gas phase	£2 00	52.20	0.50	ECCALADOS
$C_p^{\circ} = S^{\circ} =$	151.71 258.61	151.45 255.43	0.26 3.18	47TOD/OLI 47TOD/OLI	$\Delta_{\rm f}H^{\circ} = C_{\rm p}^{\bullet} =$	-53.89 132.38	-53.39 132.46	- 0.50 - 0.08	56CAM/ROS
$\Delta_{r}S^{\circ} =$	20.01	- 426.13	3.10	TITODIOLI	$S^{\circ} =$	380.62	379.83	~ 0.08 0.79	69STU/WES 69STU/WES
$\Delta_{\rm f}G^{\circ} =$		73.47			$\Delta_{f}S^{\circ} =$	200.02	-438.03	U. / 3	OSTO, WES
$\ln K_{\rm f} =$		-29.64			$\Delta_t G^\circ =$		77.21		
					$lnK_f =$		-31.15		
									<u></u>
trans-2-Pen		x C=(H)-(C)(C	.7)) + (2 × C =	C_5H_{10} (H)(C)), $\sigma = 9$	Liquid phas $\Delta_t H^{\bullet} =$	se 85.52	- 84.58	- 0.94	SOR A D /D COS
(2 ^ C-(1	1)3(C))+(1	~ C-(11)2(C)(C	/d// + (2 ^ Cd-	(11)(C)), 0 - 9	$C_p^{\circ} =$	- 65.52	181.87	-0.94	60BAR/ROS
	Literatur	e - Calculated	= Residual	Reference	$S^{\circ} =$		287.81		
		Culculated	110014041	11010101100	$\Delta_{\rm f}S^{\circ} =$		-530.06		
					$\Delta_{\mathbf{f}}G^{\circ} =$		73.46		
					$lnK_f =$		- 29.63		
Gas phase	-31.29	-32.76	1.47	86TRC	•				·
Gas phase $\Delta_t H^\circ =$		109.57	-1.12	69STU/WES					
$\Delta_{\mathbf{f}}H^{\circ} =$	108.45	340.67	-0.26	69STU/WES					
		270.07		•	cis-3-Hexen	e			C ₆ H
$\Delta_f H^{\circ} = C_p^{\circ} =$	108.45	-340.88					× C-(H)₂(C)(C	(a))+(2×Ca-(
$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} =$	108.45				(2 × C-(II				
$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} =$	108.45	-340.88				nsat) corr),	$\sigma = 18$		
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t =$	108.45 340.41	- 340.88 68.87				nsat) corr),	$\sigma = 18$ e – Calculated:	= Residual	Reference
$\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phas	108.45 340.41	-340.88 68.87 -27.78	0.07	70000001		nsat) corr),		= Residual	Reference
$\Delta_t H^\circ = C_p^\circ = S^\circ = S^\circ = \Delta_t S^\circ = InK_t = Ink_$	108.45 340.41 se - 57.98	-340.88 68.87 -27.78	0.87	79GOO/SMI	(1×cis (u	nsat) corr),		= Residual	Reference
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t = InK_t = Liquid phase \Delta_t H^\circ = C_p^\circ = InK_t = $	108.45 340.41 se -57.98 156.98	-340.88 68.87 -27.78 -58.85 151.45	5.53	47TOD/OLI	(1×cis (u	nsat) corr), Literatur	e – Calculated		
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	108.45 340.41 se - 57.98	-340.88 68.87 -27.78 -58.85 151.45 255.43			$(1 \times cis)$ Gas phase $\Delta_t H^\circ =$	Literatur	e – Calculated – 48.79	1.18	56CAM/ROS
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = $	108.45 340.41 se -57.98 156.98	-340.88 68.87 -27.78 -58.85 151.45 255.43 -426.13	5.53	47TOD/OLI	Gas phase $\Delta_t H^\circ = C_p^\circ =$	Literatur - 47.61 123.64	e – Calculated – 48.79 122.17	1.18 1.47	56CAM/ROS 69STU/WES
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = In K_t = $ Liquid pha: $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S_t G^\circ = S^\circ = S_t G^\circ = S^\circ = S_t G^\circ = S^\circ = S^\circ = S_t G^\circ = S^\circ = S_t G^\circ = S^\circ = S^\circ = S^\circ = S_t G^\circ = S^\circ = S^\circ = S_t G^\circ = S^\circ = S^\circ = S_t G^\circ = $	108.45 340.41 se -57.98 156.98	-340.88 68.87 -27.78 -58.85 151.45 255.43 -426.13 68.20	5.53	47TOD/OLI	$(1 \times cis)$ Gas phase $\Delta_t H^\circ = C_t^\circ = S^\circ = $	Literatur	e – Calculated - 48.79 122.17 378.17	1.18	56CAM/ROS
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = $	108.45 340.41 se -57.98 156.98	-340.88 68.87 -27.78 -58.85 151.45 255.43 -426.13	5.53	47TOD/OLI	Gas phase $\Delta_t H^\circ = C_p^\circ =$	Literatur - 47.61 123.64	e – Calculated – 48.79 122.17	1.18 1.47	56CAM/ROS 69STU/WES

 C_7H_{14}

C8H16

Reference

Reference

TABLE 7. n-Alkenes	(16) -	Continued
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TABLE 7. n-Alkenes (32) - Continued

		$\times C - (H)_2(C)(C)$ $\sigma = 18$	(C_d)) + (2 × C_d -(C ₆ H ₁₂ (H)(C))+	trans - 2-Hep (2 × C-(I (2 × C _d -($H_{3}(C))+(2$	\times C-(H) ₂ (C) ₂) +	- (1 × C(H) ₂	(C)(C _d))+
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated =	= Residual	Referen
Liquid pha	se				Gas phase				
$\Delta_i H^\circ =$	−78.95	- 79.31	0.36	60BAR/ROS	$\Delta_{\rm f}H^{\circ} =$	−73.54	−74.02	0.48	86TRC
$C_p^{\circ} =$		180.74			$C_{\rho}^{\circ} =$		155.35		
S° =		287.10							
$\Delta_f S^\circ =$		- 530.77							
$\Delta_t G^{\circ} =$		78.94			Liquid pha				
$lnK_f =$		-31.84			•	- 109.54	-110.31	0.77	76GOO
					$C_p^{\circ} =$		212.29		
					<i>S</i> ° =		320.19		
					$\Delta_{\mathbf{f}}S^{\circ} =$		- 633.99		
trans -3-He				C ₆ H ₁₂	$\Delta_f G^\circ =$		78.71		
(2×C-()	H)₃(C))+(2	×C-(H) ₂ (C)(C	(C_d) + $(2 \times C_d -$	$(H)(C)), \sigma = 18$	$lnK_f =$		-31.75		
	Literatur	e – Calculated	= Residual	Reference					
					cis -2-Octen	e			
Gas phase					(2×C-(H	$H_{3}(C)) + (3$	\times C-(H) ₂ (C) ₂) +	$-(1\times C-(H)_2)$	$(C)(C_d)) +$
$\Delta_f H^\circ =$	- 54.43	-53.64	-0.79	56CAM/ROS	(2×C _d -(H)(C))+(1	×cis (unsat) cor	T)	
$C_p^{\circ} =$	132.84	130.20	2.64	69STU/WES					
S° =	374.84	373.11	1.73	69STU/WES		Literatu	re – Calculated =	= Residual	Referen
$\Delta_f S^\circ =$		444.76							
$\Delta_{\rm f}G^{\circ} =$		78.96							
$lnK_f =$		-31.85			Gas phase				
					$\Delta_t H^{\circ} =$		-89.80		
					$C_p^{\circ} =$		170.21		
Liquid pha	ise								

60BAR/ROS

cis-2-Heptene C7H14 $(2 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)(C_d)) +$ $(2 \times C_d - (H)(C)) + (1 \times cis (unsat) corr)$

-84.58

180.74 287.10

-530.77

73.67

-29.72

-1.48

 $\Delta_{\rm f}H^{\circ} =$

 $C_p^{\circ} = S^{\circ} =$

 $\Delta_f S^\circ =$

 $\Delta_t G^\circ =$

 $lnK_f =$

-86.06

	Reference			
Gas phase				
$\Delta_t H^{\circ} =$	69.14	-69.17	0.03	86TRC
$C_p^{\circ} =$		147.32		
Liquid pha $\Delta_{\epsilon}H^{\circ} = C_{p}^{\circ} =$		105.04 212.29	-0.10	76GOO
$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f =$		320.19 -633.99 83.98		

$\Delta_{\mathbf{f}}H^{\circ} =$		-89.80		
C _p =		170.21		
Liquid phase	÷			
$\Delta_t H^{\circ} = -$	- 135.69	- 130.77	-4.92	86PED/NAY
$C_p^{\circ} = S^{\circ} =$		242.71		
S° =		352.57		
$\Delta_f S^\circ =$		-737.92		
$\Delta_i G^\circ =$		89.24		
$lnK_t =$		- 36.00		

trans-2-Octene C8H16 $(2 \times C - (H)_3(C)) + (3 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)(C_d)) +$ $(2 \times C_d - (H)(C))$ Literature - Calculated = Residual Reference Gas phase Δ_tH° = -94.65 $C_p^{\circ} =$ 178.24 Liquid phase $\Delta_i H^{\circ} = -135.69$ -136.04 0.35 86PED/NAY $C_p^{\circ} = S^{\circ} =$ 242.71 352.57 $\Delta_f S^\circ =$ -737.92 $\Delta_{\rm f}G^{\circ} =$ 83.97 $lnK_f =$ -33.87

TABLE 7. n-Alkenes (32) - Continued

cis -3-Heptene $(2 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) + (2 \times C$	C_7H_{14}			$\times C - (H)_2(C)(C)$ $(C)_2), \sigma = 3$	(C_d)) + $(1 \times C_d -$	C ₅ H (H)(C))+
Literature – Calculated = Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = -68.75 - 69.42$ 0.67 $C_\rho^\circ = 145.06$	86TRC	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	140.67 105.44 333.46	142.17 102.34 331.24	-1.50 3.10 2.22	55FRA/PRO 69STU/WES 69STU/WES
Liquid phase $\Delta_t H^\circ = -104.35 -105.04 0.69$ $C_p^\circ = 211.16$	76GOO	$\Delta_{f}S^{\circ} = \\ \Delta_{f}G^{\circ} = \\ \ln K_{f} = $		-219.75 207.69 -83.78		
$S^{\circ} = 319.48$ $\Delta_t S^{\circ} = -634.70$ $\Delta_t G^{\circ} = 84.19$ $\ln K_t = -33.96$		Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ$	e 150.83 244.97	114.14 148.78 244.13 - 306.85	2.05 0.84	70TOD/MES 70TOD/MES
trans-3-Heptene $(2 \times C-(H)_3(C)) + (1 \times C-(H)_2(C)_2) + (2 \times C-(H)_2(C)_2) + (2 \times C-(H)_2(C)_2)$ $(2 \times C_d-(H)(C))$	C_7H_{14} $C_7(C_d)$ +	$\Delta_t G^\circ = \\ \ln K_t = \\ -$		205.63 - 82.95		
Literature – Calculated = Residual	Reference	1,3-Butadien (2×C _d -(F		C _d -(H)(C _d)), σ	= 2	C₄H
Gas phase $\Delta_t H^\circ = -73.73 -74.27$ 0.54 $C_n^\circ = 153.09$	86TRC		Literatur	e – Calculated	= Residual	Reference
Liquid phase $ \Delta_t H^\circ = -109.33 -110.31 0.98 $ $ C_\rho^\circ = 211.16 $ $ S^\circ = 319.48 $ $ \Delta_t S^\circ = -634.70 $ $ \Delta_t G^\circ = 78.92 $ $ \ln K_f = -31.84 $	76GOO	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{1}{2}$	108.82 79.54 278.74	109.20 79.84 280.76 - 133.92 149.13 - 60.16	- 0.38 - 0.30 - 2.02	49PRO/MAR 69STU/WES 69STU/WES
1,2-Butadiene $(1 \times C_{-}(H)_{3}(C)) + (1 \times C_{d}-(H)(C)) + (1 \times C_{a}) + (1 \times C_{a})$	C_4H_6 C_{α} - $(H)_2$), $\sigma = 3$		(C))+(1×0	C _d -(H)(C)) + (2 (unsat) corr), c		C_5H (1 × C_{d} ~(H) ₂)
Literature – Calculated = Residual	Reference			e – Calculated		Reference
Gas phase $ \Delta_t H^\circ = 162.26 163.05 -0.79 $ $ C_p^\circ = 80.12 81.71 -1.59 $ $ S^\circ = 293.01 293.04 -0.03 $ $ \Delta_t S^\circ = -121.64 $ $ \Delta_t G^\circ = 199.32 $ $ \ln K_t = -80.40 $	49PRO/MAR 69STU/WES 69STU/WES	Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f = $	82.76 94.56 324.26	81.79 94.90 327.30 -223.69 148.48 -59.90	0.97 - 0.34 - 3.04	55FRA/PRO 69STU/WES 69STU/WES
		Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ - \Delta_t G^\circ = \ln K_t =$	e	54.82 152.79 224.67 - 326.31 152.11 - 61.36		Allasta, respi

C₅H₈

C₅H₈

 $\Delta_t G^\circ =$

 $lnK_f =$

TABLE 7. n-Alkenes (16) - Continued

Table 7. n-A	lkenes (32) -	 Continued
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	Literatur	Literature - Calculated = Residual				
Gas phase						
$\Delta_t H^\circ =$	75.81	76.94	-1.13	55FRA/PRO		
$C_p^{\circ} =$	103.34	102.93	0.41	69STU/WES		
S° =	319.66	322.24	- 2.58	69STU/WES		
$\Delta_f S^\circ =$		-228.75				
$\Delta_f G^\circ =$		145.14				
$lnK_f =$		- 58.55				
Liquid pha	se					
$\Delta_t H^\circ =$		49.55				
$C_p^{\circ} =$		152.79				
S° =		224.67				
$\Delta_f S^\circ =$		-326.31				
$\Delta_{\rm f}G^{\circ} =$		146.84				
$lnK_f =$		- 59.23				

	Literatur	e – Calculated =	Reference	
Gas phase			·	
$\Delta_t H^\circ =$	106.36	106.36	0.00	55FRA/PRO
$C_p^{\circ} =$	105.02	105.01	0.01	69STU/WES
S° =	333.46	333.46	0.00	69STU/WES
$\Delta_f S^\circ =$		-217.53		
$\Delta_f G^{\circ} =$		171.22		
$lnK_f =$		- 69.07		***************************************
Liquid pha	se			
$\Delta_t H^\circ =$	81.17	81.17	0.00	86TRC
$C_p^{\circ} =$	146.82	146.82	0.00	70MES/TOD
<i>S</i> ° =	248.86	248.86	0.00	70MES/TOD
$\Delta_f S^\circ =$		-302.12		
$\Delta_f G^\circ =$		171.25		
$lnK_f =$		- 69.08		

1,4-Pentadiene

2,3-Pentadiene

$(2 \times C_{-}(H)_{3}(C)) + (2 \times C_{d}(H)(C)) + (1 \times C_{a}), \sigma = 18$						
	Literatur	Reference				
Gas phase						
$\Delta_i H^{\circ} =$	133.05	130.79	2.26	55FRA/PRO		
$C_p^{\circ} =$	101.25	104.80	-3.55	69STU/WES		
<i>S</i> ° =	324.68	322.99	1.69	69STU/WES		
$\Delta_f S^\circ =$		- 228.00				
$\Delta_f G^\circ =$		198.77				
$lnK_f =$		-80.18				

,	iene (Contin H)3(C))+(2:	,	+ (1×C _a), σ =	C ₅ H ₂ = 18		
	Literatur	Literature – Calculated = Residual				
Liquid pha	ise					
$\Delta_f H^\circ =$	103.55	101.56	1.99	70MES/TOD		
$C_p^{\circ} =$	152.34	152.20	0.14	70MES/TOD		
S° =	237.32	238.15	-0.83	70MES/TOD		
$\Delta_{\mathbf{r}}S^{\circ} =$		-312.83				
$\Delta_{\mathbf{f}}G^{\circ} =$		194.83				
$lnK_f =$		- 78.59 				
Allene				С₃Н		
$(1 \times C_a)$	$+(2\times C_d-(H))$	$)_2), \sigma = 4$				
	Literatur	e – Calculated	= Residual	Reference		
Gas phase						
$\Delta_{\rm f} H^{\circ} =$	191.25	195.31	-4.06	36KIS/RUH2		
$C_p^{\circ} =$	58.99	58.62	0.37	69STU/WES		
S° =	243.93	245.79	-1.86	69STU/WES		
$\Delta_f S^\circ =$		-32.57				

205.02

-82.70

TABLE 8. s-Alkenes (34)

	[)₃(C))+(1>	$(C_{d}-(H)_2)+(1$ ary)), $\sigma = 18$	$\times C_{d}$ - $(C)_{2}$ +	C₄H ₈		$H_{3}(C)) + (1$	$\times C_d$ –(H)(C))- iary)), $\sigma = 9$	+ (1 × C _d -(C) ₂)	C ₅ H ₁₀)+
	Literatur	e – Calculated =	= Kesidual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = C_p^\circ$	-17.87 89.12	- 18.58 87.94	0.71 1.18	51PRO/MAR 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ =$	-41.00 105.02	-50.84 111.03	9.84 6.01	49SCO/WAD 69STU/WES
$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f =$	293.59	295.29 - 249.96 55.94 - 22.57	-1.70	69STU/WES	$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f =$	338.57	345.90 - 335.65 49.24 - 19.86	-7.33	69STU/WES
2 Mathyl 1	hutono			СЧ	Liquid pha Δ _t H° =		76.00	0.01	70COO/EM
	$H_{3}(C) + (1 + 1)_{2}(C)(C_{d})$	$\times C_{d}$ -(H) ₂)+(1 +(1×-CH ₃ cor	rr (tertiary)),		$C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} =$	- 68.07 152.80 251.04	-76.98 157.26 248.65 -432.90	8.91 -4.46 2.39	79GOO/SMI 47TOD/OLI 47TOD/OLI
	Literatur	e Calculated :	= Residual	Reference	$\Delta_f G^\circ = \ln K_f =$		52.09 -21.01		
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	-35.10 111.63 339.53	- 37.20 108.57 339.25 - 342.30	2.10 3.06 0.28	86TRC 69STU/WES 69STU/WES		H)₃(C))+(1	×C-(H) ₂ (C)(0 -CH ₃ corr (tert		C₄H ₁₂ (H)(C))+
$\Delta_f G^\circ = \ln K_f =$		64.86 26.16				Literatu	re – Calculated	= Residual	Reference
Liquid phas	se	77 p. 3 a siste a si 0 2 a si 1 a			Gas phase				
$\Delta_t H^\circ = C_p^\circ = S^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{1}{2}$	- 60.96 157.19 253.97	- 62.22 153.84 254.63 - 426.92 65.07 - 26.25	1.26 3.35 -0.66	79GOO/SMI 47TOD/OLI 47TOD/OLI	$ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	- 66.86 126.61 378.44	-71.72 131.66 384.10 -433.76 57.61 -23.24	4.86 - 5.05 - 5.66	56CAM/ROS 69STU/WES 69STU/WES
2-Methyl-1- (2×C-(I (1×C _d -(σ = 9	$H_{3}(C)) + (1$	× C-(H) ₂ (C) ₂) C _d -(H) ₂) + (1×	+(1×C−(H) ₂ −CH ₃ corr (te	$C_{\epsilon}H_{12}$ (C)(C _d)) + rtiary)),	Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \Delta_t G^\circ = S^\circ $	se - 98.53	- 102.71 186.55 280.32 - 537.55 57.56	4.18	60BAR/ROS
	Literatur	re – Calculated	= Residual	Reference	$\ln K_{\rm f} =$		-23.22		
Gas phase $ \Delta_t H^\circ = \\ C_p^\circ = \\ S^\circ = \\ \Delta_r S^\circ - $	- 59.37 135.60 382.17	- 57.83 131.46 378.41 439.45	-1.54 4.14 3.76	56CAM/ROS 69STU/WES 69STU/WES			×C−(H)₂(C)(C	C _d))+(1×C _d -(C ₆ H ₁₂ (C) ₂) +
$\Delta_f G^\circ = \ln K_f =$		73.19 - 29.53				Literatu	re – Calculated	= Residual	Reference
Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	se 89.96	87.95 184.26 287.01 530.86 70.32 28.37	- 2.01	60BAR/ROS	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ - \Delta_t G^\circ = \ln K_t =$	- 56.02 133.55 376.60	-55.82 129.20 371.69 -446.18 77.21 -31.15	-0.20 4.35 4.91	56CAM/ROS 69STU/WES 69STU/WES

(2×C-(H	utene (Conti $H_{3}(C)$) + (2: H_{2}), $\sigma = 1$	< C-(H)2(C)(C	(d) + $(1 \times C_d - (1 \times C_d))$	(C_6H_{12})	(1×C-(H	H) ₃ (C)) + (1 H) ₂ (C)(C _d))	\times -CH ₃ corr (t + (1 \times C _d -(C) ₂		C ₆ H ₁₂ sat) corr)+
	Literatur	e – Calculated :	= Residual	Reference	(1×Ca-(H)(C)), σ =	= 27 re – Calculated	= Residual	Reference
Timuid abov						***************************************			
Liquid phas $\Delta_t H^\circ =$	se -87.11	- 85.77	- 1.34	60BAR/ROS	Gas phase				
$C_p^{\circ} =$		183.13			$\Delta_f H^{\circ} =$	-62.30	- 64.61	2.31	56CAM/ROS
<i>S</i> ° =		286.30			$C_p^{\circ} =$	126.61	123.63	2.98	69STU/WES
$\Delta_f S^\circ =$		-531.57			S° =	378.44	380.03	- 1.59	69STU/WES
$\Delta_f G^\circ =$		72.72			$\Delta_{\mathbf{f}}S^{\circ} =$		- 437.84		
$lnK_{f} =$		- 29.33			$\Delta_{\mathbf{f}}G^{\circ} =$		65.93		
					$lnK_f =$		- 26.60		
3-Methyl-1-	-butene			C ₅ H ₁₀	Liquid phas	se			
•		× C-(H)(C)₂(C	(_d))+		$\Delta_{\rm f}H^{\circ} =$	- 94.47	- 95.26	0.79	60BAR/ROS
		$(1 \times C_d$		•	$C_p^{\circ} =$		186.55		
(1×C _d −($H)_2$), $\sigma = 9$)			<i>s</i> ° =		280.32		
					$\Delta_{i}S^{\circ} =$		-537.55		
	Literatur	e – Calculated:	= Residual	Reference	$\Delta_{\mathbf{r}}G^{\circ} =$		65.01		
					$lnK_f =$		-26.22		
Gas phase $\Delta_t H^\circ =$	-27.75	- 28.03	0.28	86TRC					
$C_p^{\circ} =$	118.62	119.07	-0.45	69STU/WES	trans -3-Met	hvl-2-pente	ne		C ₆ H ₁₂
$S^{\circ} =$	333.46	334.56	-1.10	69STU/WES			 × C-(H)₂(C)(0	Ca))+	CSIII
$\Delta_{\mathbf{f}}S^{\circ} =$	555.10	- 346.99					$(1 \times C_{\rm dr})$,	
$\Delta_{\rm f}G^{\circ} =$		75.43				H)(C)), \sigma =		(0)2)	
$\ln K_{\rm f} =$		- 30.43			(21150)	/(-//, -			
						Literatur	e – Calculated	= Residual	Reference
Liquid pha		£1 00	0.20	70GOO/SMI	Goa mhosa				
$\Delta_{f}H^{\circ} =$	-51.60	-51.80 156.05	0.20 0.01	79GOO/SMI 47TOD/OLI	Gas phase $\Delta_f H^\circ =$	-63.14	- 69.46	6.32	56CAN(DO0
$C_p^{\circ} = S^{\circ} =$	156.06 253.30	253.30	0.00	47TOD/OLI	$C_p^{\circ} =$	126.61	131.66	- 5.05	56CAM/ROS 69STU/WES
$\Delta_{f}S^{\circ} =$	233.30	- 428.26	0.00	4/10D/OLI	S° =	381.83	374.97	6.86	69STU/WES
$\Delta_{\rm f}G^{\circ} =$		75.88			$\Delta_{\rm f} S^{\circ} =$	501.05	- 442.90	0.00	0931 U/ WES
$\ln K_{\rm f} =$		-30.61			$\Delta_{r}G^{\circ} =$		62.59		
		· · · · · · · · · · · · · · · · · · ·			$lnK_f =$		-25.25		
2 Maded 1	4			C ₆ H ₁₂	Tiavid shar				
3-Methyl-1-	-	× C-(H) ₂ (C) ₂)	+ (1 × C-/H)(Liquid phas $\Delta_t H^\circ =$	- 94.56	- 100.53	5.97	60BAR/ROS
		$(11)_2(C)_2$ ary)) + $(1 \times C_{d}$		C)2(Ca)) 1	$C_p^{\circ} =$	74.50	186.55	3.31	ODAK/KOS
	$(H)_2$), $\sigma = 9$		(11)(0))		S° =		280.32		
(17,00)	(11)2), 0	,			$\Delta_{f}S^{\circ} =$		-537.55		
	Literatur	e - Calculated	= Residual	Reference	$\Delta_{r}G^{\circ} =$		59.74		
					$\ln K_f =$		-24.10		
Gas phase			_						
$\Delta_{\rm f}H^{\circ} =$	-49.50	46.40	-3.10	56CAM/ROS					
$C_{\rho}^{\circ} =$	142.42	141.96	0.46	69STU/WES	3-Methyl-cis				C7H14
S° =	376.81	373.72	3.09	69STU/WES			×-CH ₃ corr (t		
$\Delta_f S^\circ = \Delta_f $		444.14 96.00					$+(1\times C_{d}-(H)($	$(1) + (1 \times cis)$	insat) corr)+
$\Delta_f G^\circ =$		86.02			$(1 \times C_d - (0))$	C) ₂)			
$lnK_f =$		-34.70				Literatur	e – Calculated	= Residual	Reference
Liquid pha	se								
$\Delta_t H^{\circ} =$	-78.16	-75.35	-2.81	60BAR/ROS	Gas phase				
$C_p^{\circ} =$		186.47			$\Delta_{\mathbf{f}}H^{\circ} =$	−79.41	-85.49	6.08	60CAM/ROS
S° =		285.68			$C_{\rho}^{\circ} =$		144.26		
$\Delta_f S^{\circ} =$		-532.19			-		·		
$\Delta_l G^{\circ}$ –		83.32							
$lnK_f =$		-33.61							

TABLE 8. s-Alkenes (34) - Continued

3-Methyl-cis-3-hexene (Continued) $(3 \times C - (H)_3(C)) + (1 \times -CH_3 \text{ corr (tertiary)}) + (1 \times -CH_3 \text{ corr} (H)_3(C)) + (1 \times -CH_3 \text{ corr})$	C ₇ H ₁₄	cis-4-Methy (3×C-(H (2×-CH)	$H_{3}(C)) + (2)$	× C _d ~(H)(C)) - ary)) + (1 × cis	+ (1 × C-(H)(0 (unsat) corr),	$C_{\epsilon}H_{12}$ $C_{2}(C_{d})) + \sigma = 27$
$(2 \times C_{-}(H)_{2}(C)(C_{d})) + (1 \times C_{d}-(H)(C)) + (1 \times cis (unside (1 \times C_{d}-(C)_{2}))$	it) corr) +		Literature	e – Calculated	= Residual	Reference
Literature – Calculated = Residual	Reference	Gas phase			· · · · · · · · · · · · · · · · · · ·	
Liquid phase $\Delta_{\ell}H^{\circ} = -115.94 -120.99$ 5.05 $C_{\rho}^{\circ} = 215.84$ $S^{\circ} = 311.99$ $\Delta_{\ell}S^{\circ} = -642.19$ $\Delta_{\ell}G^{\circ} = 70.48$ $\ln K_{\ell} = -28.43$	61ROC/ROS	$ \Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = $	-57.49 133.55 373.34	- 55.44 134.13 375.34 - 442.53 76.50 - 30.86	- 2.05 - 0.58 - 2.00	56CAM/ROS 69STU/WES 69STU/WES
3-Methyl-trans-3-hexene $(3 \times C - (H)_3(C)) + (1 \times -CH_3 \text{ corr (tertiary)}) + (2 \times C - (H)_2(C)(C_d)) + (1 \times C_d - (H)(C)) + (1 \times C_d - (C))$	•	Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f =$	se -87.03	-84.84 188.76 278.99 -538.88 75.83 -30.59	-2.19	60BAR/ROS
Literature — Calculated = Residual	Reference					
Gas phase $\Delta_t H^{\circ} = -76.82 -90.34$ 13.52 $C_p^{\circ} = 152.29$	60CAM/ROS		$H_{3}(C)) + (2)$	ne ×-CH ₃ corr (t + (2×C _d -(H)(C ₆ H ₁₂
Liquid phase			Literature	e – Calculated	= Residual	Reference
$\Delta_t H^\circ = -112.72$	61ROC/ROS	Gas phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-61.50 141.42 368.28	-60.29 142.16 370.28 -447.59 73.16 -29.51	- 1.21 - 0.74 - 2.00	56CAM/ROS 69STU/WES 69STU/WES
4-Methyl-1-pentene $(2 \times C - (H)_3(C)) + (1 \times C - (H)(C)_3) + (2 \times -CH_3 \text{ corr } (1 \times C - (H)_2(C)(C_d)) + (1 \times C_d - (H)_2) + (1 \times C_d - (H)(C)(C_d))$)), $\sigma = 9$	Liquid phas $ \Delta_t H^{\circ} = C_p^{\circ} = $	se 91.55	- 90.11 188.76	- 1.44	60BAR/ROS
Literature - Calculated = Residual Gas phase	Reference	$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f =$		278.99 538.88 70.56 28.46		
$\Delta_t H^\circ = -51.25 -48.45 -2.80$ $C_p^\circ = 126.48 132.29 -5.81$ $S^\circ = 367.73 369.54 -1.81$ $\Delta_t S^\circ = -448.32$ $\Delta_t G^\circ = 85.22$ $\ln K_f = -34.38$	56CAM/ROS 69STU/WES 69STU/WES	(3×-CH	I) ₃ (C)) + (1 > corr (quate	ne × C-(C)3(Cd)) ernary)) + (1 × × t-butyl cis co	$C - (H)_2(C)(C_0)$	C ₈ H ₁₆
Liquid phase $\Delta_t H^\circ = -80.04 -77.28 -2.76$	60BAR/ROS	·	Literature	e – Calculated	= Residual	Reference
$C_p^o = -80.04 - 77.28 - 2.76$ $C_p^o = 176.60$ $S^o = 289.15$ $\Delta_t S^o = -528.72$ $\Delta_t G^o = 80.36$ $\ln K_t = -32.42$	WILKINGS	Gas phase $\Delta_t H^\circ = C_\rho^\circ =$	-89.29	- 91.59 170.19	2.30	60CAM/ROS

TABLE 8.	s-Alkenes	(34) -	Continued
I ADLL U	2 THEFIT	(-,	Commen

$(1 \times C - (C)_3(C_d))$	+	C ₈ H ₁₆	(4×C-(H	$I_{3}(C) + (2$	- ' '-'		C ₆ H ₁₂
		d <i>))</i>		Literatu	re – Calculated	= Residual	Reference
ture – Calculated	= Residual	Reference				-	
- 128.97 253.15 313.83 -776.66 102.59 -41.38	2.53	61ROC/ROS	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-69.79 123.60 364.64	-89.80 133.12 365.30 -452.57 45.13 -18.21	20.01 - 9.52 - 0.66	56CAN/ROS 69STU/WES 69STU/WES
					120.84	18.42	60BAR/ROS
$(1 \times C - (C)_3(C_d))$ uaternary)) + $(2 \times$		CgH ₁₆	$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f = 0$	174.68 270.20	192.36 273.54 - 544.33 41.45 - 16.72	- 17.68 - 3.34	55SCO/FIN 55SCO/FIN
nture – Calculated	= Residual	Reference					
5 - 108.83 170.19	1.18	60CAM/ROS	(3×C-(H	$I_{3}(C)+(1$	\times C-(H)(C) ₃)+		
				Literatur	e – Calculated :	= Residual	Reference
253.15 313.83 -776.66	1.52	61ROC/ROS	Gas phase $\Delta_t H^\circ = C_p^\circ =$	-83.81	- 85.15 154.38	1.34	60CAM/ROS
85.11 -34.33			$\Delta_t H^\circ =$		- 118.96 211.70	1.98	61ROC/ROS
$+(1\times C-(H)(C)_2(C)$	(C_d)) + $(1 \times C_{d}$ — (tiary)), $\sigma = 2$	C_6H_{12} (C) ₂) +	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$		314.04 - 640.14 71.90 - 29.00		
ature – Calculated	= Residual	Reference					
7 141.16	-1.63 2.31	56CAM/ROS 69STU/WES	(4×C-(H	I) ₃ (C))+(1 corr (terti	\times C-(H)(C) ₂ (C _d ary)) + (1 \times C _d -	(H)(C))+(1>	
- 449.01	-3.22	69STU/WES		Literatur	e – Calculated =	= Residual	Reference
- 27.89			Gas phase $\Delta_t H^\circ =$	88.70	-99.25	10.55	60CAM/ROS
191.15	-2.12	60BAR/ROS	Liquid phas			10.00	(1000707
278.19 539.68 67.42 27.20			$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	123.09	-133.97 223.86 303.88 -650.30	10.88	61ROC/ROS
	(1 × C-(C) ₃ (C _d)) - uaternary) + (1 × (1 × t-butyl cis conture - Calculated cis conture - C	ture - Calculated = Residual 1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	exene (Continued) $(1 \times C - (C)_3(C_3)) + (1 \times C - (C)_3(C_3)) + (1$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Capting Cap	C_4H_4 (1×C-(C)(C_4)) + (2×C_+(C)(C_4)) + (1×C-(C)(C_4)) + (1×C-(C)(C_4

TABLE 8. s-Alkenes (34) - Continued

(3×-CH₃	() ₃ (C))+(1>	× C-(C) ₃ (C _d)) - ernary)) + (1 ×		C_6H_{12}	(4×C-(I	$H_{3}(C) + (1$	entene (Contin × C-(C) ₃ (C _d)) ternary)) + (2×	+	C7H14
(1×C _d -(1		e – Calculated	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-61.59 126.48 343.76	-55.69 126.47 343.76 -474.10 85.66 -34.56	- 5.90 0.01 0.00	56CAM/ROS 69STU/WES 69STU/WES	Liquid phant $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = 0$	se - 121.71	- 120.72 223.86 282.16 - 672.02 79.64 - 32.13	- 0.99	61ROC/ROS
Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se - 88.28 191.17 256.50	-82.41 191.15 256.47 -561.40 84.97 -34.28	-5.87 0.02 0.03	60BAR/ROS 38KEN/SHO 38KEN/SHO	(4×C-(I (3×-CH	I ₃ corr (quat I ₃ corr (terti	the \times C-(C) ₃ (C _d)) ternary))+(1×C _d -ary))+(1×C _d -ce-Calculated	C_{d} -(C) ₂) + -(H) ₂)	C₁H₁₄ Reference
cis -4,4-Dime	I) ₃ (C))+(1	iene × C-(C)3(C _d))		C ₇ H ₁₄	Gas phase $\Delta_t H^\circ = C_p^\circ =$	-85.48	- 92.39 148.56	6.91	60CAM/ROS
	yl cis corr)	ernary)) + (2 ×		Reference	Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \Delta_t G^\circ = S^\circ = S^\circ$	se 117.70	-124.09 226.25 281.36 -672.82 76.51	6.39	61ROC/ROS
$\Delta_{i}H^{\circ} = C_{p}^{\circ} =$	-72.63	- 70.71 149.56	-1.92	60CAM/ROS	$lnK_f =$		-30.86		
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \Delta_t G^\circ$	se - 105.31	-103.24 223.86 282.16 -672.02 97.12	- 2.07	61ROC/ROS	(4×C-(I (4×-CH	3 corr (terti insat) corr)	ene × C-(H)(C) ₂ (C ary)) + (2 × C _d - e – Calculated	-(H)(C))+	C₂H₁₀ Reference
	1)₂(C))+(1	-39.18 entene $\times C - (C)_3(C_4))$ ternary)) + (2 ×		C7H14	Gas phase $\Delta_t H^\circ = C_p^\circ =$		- 103.85 187.35		
	Literatur	re – Calculated	= Residual	Reference	Liquid phas $\Delta_t H^\circ = C_{t'}^\circ =$	se 151.08	-141.83 255.36	-9.25	73YAT/MCD
Gas phase $\Delta_t H^\circ = C_\rho^\circ =$	-88.78	- 87.95 149.56	-0.83	60CAM/ROS	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}K_{t} - \Delta_{t}K_{t}$	·	334.22 -756.27 83.65 -33.74		

69.00

-27.83

-783.44

 $\Delta_f S^{\circ} =$

 $\Delta_f G^\circ =$

 $lnK_f =$

TABLE 8. s-Alkenes (34) - Continued

······································						
trans-2,5-Dimethyl-3-hexene $(4 \times C-(H)_3(C)) + (2 \times C-(H)(C)_2(C_d)) + (4 \times -CH_3 \text{ corr (tertiary)}) + (2 \times C_d-(H)(C))$	C ₈ H ₁₆	(3×C-(I		tene \times C-(H) ₂ (C) ₂) - C_d -(H) ₂) + (1 \times -		
Literature - Calculated = Residual	Reference	Literature - Calculated = Residual Refere				
Gas phase		Gas phase				
$\Delta_t H^\circ = -108.70$		$\Delta_t H^\circ =$	-100.29	- 101.47	1.18	60CAM/ROS
$C_p^{\circ} = 195.38$	·/-	$C_p^{\circ} =$	2002	186.94	2.20	0001111/1100
Liquid phase	,	Liquid pha	Se Se			
$\Delta_t H^\circ = -159.28 -147.10 -12.18$	73YAT/MCD	$\Delta_t H^\circ =$	- 136.36	- 140.58	4.22	61ROC/ROS
$C_p^0 = 255.36$	15 17 17 MCD	$C_p^{\circ} =$	150.50	251.99	7.22	UNCCROS
$S^{\circ} = 334.22$	4	$S^{\circ} =$		342.95		
$\Delta_{i}S^{\circ} = -756.27$		$\Delta_f S^\circ =$		- 747 . 54		
$\Delta_{0} = -730.27$		$\Delta_{\mathbf{f}}G^{\circ} =$		82.30		
$\Delta_t G^{\circ} = 78.38$ $\ln K_f = -31.62$		$\ln K_{\rm f} =$		- 33.20		
2,4,4-Trimethyl-1-pentene	C ₈ H ₁₆		-ethyl-1-bute			C ₇ H ₁₄
$(4 \times C-(H)_3(C)) + (1 \times C-(C)_4) + (3 \times -CH_3 \text{ cor} (1 \times C-(H)_2(C)(C_d)) + (1 \times C_d-(C)_2) + (1 \times$		(3×C-(1 (2×-CH (1×C _d -(3 corr (tertia	× C-(H)(C) ₂ (C _e ary)) + (1 × C-(i	₁)) + H) ₂ (C)(C _d)) -	$+(1\times C_{d}-(C)_{2})+$
Literature Calculated = Residual	Reference		Literatur	e – Calculated =	= Residual	Reference
Gas phase		Gas phase				
$\Delta_t H^{\circ} = -110.37 -116.20$ 5.83	60CAM/ROS	$\Delta_l H^\circ =$	-79.54	-83.35	3.81	60CAM/ROS
$C_p^{\circ} = 176.56$		$C_p^{\circ} =$		161.79		
Liquid phase		Liquid pha	Se.			
$\Delta_t H^\circ = -146.15 - 152.62 6.47$	61ROC/ROS	$\Delta_{f}H^{\circ} =$	– 114.06	-117.03	2.97	61ROC/ROS
$C_p^0 = 240.20$ 237.04 3.16	36PAR/TOD2	$C_p^{\circ} =$	-114.00	220.44	2.91	OIKOC/KOS
$S^{\circ} = 311.71 322.58 -10.87$	36PAR/TOD2	$S^{\circ} =$		309.86		
$\Delta_{c}S^{\circ} = -767.91$	30FAR/10D2	$\Delta_f S^\circ =$		-644.32		
$\Delta_{\mathbf{f}}\mathbf{G}^{\circ} = 76.33$		$\Delta_f G^\circ =$		75.07		
$\ln K_{\rm f} = -30.79$		$\ln K_{\rm f} =$		-30.28		
2,4,4-Trimethyl-2-pentene $(5 \times C-(H)_3(C)) + (1 \times C-(C)_3(C_d)) +$	C ₈ H ₁₆		3-butadiene 1) ₃ (C)) + (2>	< C _d −(H) ₂) + (1	× C4-(H)(C4	C ₅ H ₈
$(3 \times -CH_3 \text{ corr (quaternary)}) + (1 \times C_d - (H)(C)$ $(2 \times -CH_3 \text{ corr (tertiary)})$	$+(1\times C_{d}-(C)_{2})+$	(1×C _d -($C)(C_d))+(1$	×-CH ₃ corr (to	ertiary)), $\sigma =$	= 3
Literature – Calculated = Residual	Reference		Literature	e – Calculated =	Residual	Reference
Exertine Calculated - Residual		Gas phase				
		$\Delta_{\mathbf{f}}H^{\circ} =$	75.73	73.18	2.55	55FRA/PRO
Gas phase		$C_p^{\circ} =$	104.60	104.60	0.00	69STU/WES
$\Delta_i H^\circ = -104.89 - 126.91$ 22.02	60CAM/ROS	S° =	315.64	315.64	0.00	69STU/WES
$C_p^{\circ} = 171.65$		$\Delta_{\mathbf{f}}S^{\circ} =$		-235.35	2.00	
		$\Delta_{\mathbf{f}}G^{\circ} =$		143.35		
		$\ln K_{\rm f} =$		-57.83		
Liquid phase						
$\Delta_t H^\circ = -142.42 - 164.58$ 22.16	61ROC/ROS	Liquid phas	se.			
$C_p^{\circ} = 258.96$		$\Delta_{\rm f}H^{\circ} =$	48.95	46.31	2.64	36BEK/WOO
$S^{\circ} = 307.05$		$C_n^{\circ} =$	151.08	151.08	2.04 0.00	70MES/TOD
4.00		Un -	1.71.00	1.21.00	U.LEJ	(UNVICA/ILLI)

 $C_p^{\circ} = S^{\circ} =$

 $\Delta_f S^{\circ} =$

 $\Delta_i G^{\circ} =$

 $lnK_f =$

151.08

228.28

151.08

227.06

-323.92

142.89

-57.64

0.00

1.22

70MES/TOD

70MES/TOD

TABLE 8. s-Alkenes (34) - Continued

TABLE 9. Alkynes (28)

	1) ₂) + (1 × C	– Calculated =	- Desidual	Reference		Literatur	e – Calculated	= Residual	Reference
	Literature		- Residual					 	
Gas mbasa					Gas Phase $\Delta_t H^\circ =$	228.19	227.00	1 10	2000014716
$\Delta_t H^\circ =$	129.08	124.09	4.99	86TRC	$C_p^{\circ} =$	43.93	45.10	1.19	39CON/KIS
$C_p^{\circ} =$	105.44	103.80	1.64	69STU/WES	$S^{\circ} =$	200.83	198.16	-1.17 2.67	69STU/WES
$S^{\circ} =$	319.66	321.57	- 1.91	69STU/WES	$\Delta_f S^\circ =$	200.63		2.07	69STU/WES
$\Delta_{f}S^{\circ} =$	319.00		- 1.91	09310/WE3	$\Delta_{f}G^{\circ} =$		56.11		
		-229.42 192.49			-		210.27 84.82		
$\Delta_f G^\circ = \ln K_f =$		- 77.65			$lnK_f =$		- 64.62		
Liquid phas					Propyne				C ₃ I
$\Delta_{\mathbf{f}}H^{\circ} =$	101.17	96.01	5.16	69GOO2	(1×C-(F	I)₃(C))+(1	\times C ₁ -(C)) + (1	×C₁−(H)), σ :	= 3
$C_p^{\circ} =$	152.42	154.59	-2.17	70MES/TOD					
S° =	231.79	237.35	-5.56	70MES/TOD		Literatur	e – Calculated	= Residual	Reference
$\Delta_f S^{\circ} =$		-313.63							
$\Delta_{\rm f}G^{\circ} =$		189.52							
$lnK_f =$		- 76.45			Gas Phase				
					$\Delta_f H^\circ =$	184.93	186.34	- 1.41	39CON/KIS
					$C_p^{\circ} =$	60.67	61.50	- 0.83	69STU/WES
					<i>s</i> ° =	248.11	246.47	1.64	69STU/WES
					A .C° -		-31.90		
2,3-Dimethy					$\Delta_f S^\circ =$		~ 31.50		
				C_6H_{10}	$\Delta_{\rm f}G^{\circ} =$		195.85		
	(C) + (2)	$\times C_{d}-(H)_{2})+(2$	$\times C_d$ -(C)(C _d)						
		$\times C_{d}-(H)_{2})+(2$	$\times C_d$ -(C)(C_d)		$\Delta_f G^\circ =$		195.85		
	I) ₃ (C)) + (2: corr (tertia	$\times C_{d}-(H)_{2})+(2$			$\Delta_f G^\circ =$		195.85		
	I) ₃ (C)) + (2: corr (tertia	× C _d (H) ₂) + (2 ary))))+	$\Delta_f G^\circ = \ln K_f = \frac{1-\text{Butyne}}{1}$	H) ₃ (C))+(1:	195.85 - 79.00		C ₄ F C))+
(2×-CH	I) ₃ (C)) + (2: corr (tertia	× C _d (H) ₂) + (2 ary))))+	$\Delta_f G^\circ = \ln K_f = \frac{1 - \text{Butyne}}{(1 \times \text{C-(F)})^{-1}}$	$H_{3}(C)$) + (1: H)), $\sigma = 3$	195.85	C ₁))+(1×C ₁ -((
(2×-CH) Gas phase	I) ₃ (C)) + (2: corr (tertia	× C _d (H) ₂) + (2 ary))))+	$\Delta_f G^\circ = \ln K_f = \frac{1 - \text{Butyne}}{(1 \times \text{C-(F)})^{-1}}$	$H)), \sigma = 3$	195.85 - 79.00		
(2×-CH) Gas phase	I) ₃ (C)) + (2: s corr (tertian Literature	× C _d -(H) ₂) + (2 ary)) e – Calculated =	= Residual	Reference	$\Delta_f G^\circ = \ln K_f = \frac{1 - \text{Butyne}}{(1 \times \text{C-(F)})^{-1}}$	$H)), \sigma = 3$	195.85 - 79.00 × C-(H) ₂ (C)(C		C))+
Gas phase $\Delta_t H^\circ = C_p^\circ =$	(I) ₃ (C)) + (2: 3 corr (tertial Literature 45.10	\times C _d -(H) ₂) + (2 ary)) e - Calculated =	= Residual	Reference	$\Delta_t G^\circ = \frac{1 \cdot Butyne}{(1 \times C - (I \cdot 1 \times C_t - ($	H)), σ = 3 Literatur	195.85 - 79.00 × C-(H) ₂ (C)(C	= Residual	C))+ Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase	I) ₃ (C)) + (2: a corr (tertial Literature 45.10	× C _d -(H) ₂) + (2 ary)) e - Calculated = 37.16 129.36	= Residual	Reference 37DOL/GRE	$\Delta_t G^\circ = \ln K_t = \frac{1 - \text{Butyne}}{1 \times C - (1 \times C_t - (1 \times C_t - (1 \times C_t + $	H)), σ = 3 Literatur	195.85 - 79.00 × C-(H) ₂ (C)(C e - Calculated	= Residual 1.41	C))+ Reference 51PRO/MAR
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$	(I) ₃ (C)) + (2: 3 corr (tertial Literature 45.10	× C _d -(H) ₂) + (2 ary)) e - Calculated = 37.16 129.36	= Residual	Reference	$\Delta_t G^\circ = \ln K_t = \frac{1 - \text{Butyne}}{1 \times C - (1 \times C_t - (1 \times C_t - (1 \times C_t + C_t)))}$ Gas Phase $\Delta_t H^\circ = C_p^\circ = \frac{1 \times C_t - (1 \times C_t - (1 \times C_t))}{1 \times C_t - (1 \times C_t - (1 \times C_t))}$	H)), σ = 3 Literatur 165.23 81.42	195.85 - 79.00 × C-(H) ₂ (C)(C e - Calculated 166.64 82.47	= Residual - 1.41 - 1.05	C))+ Reference 51PRO/MAR 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$	I) ₃ (C)) + (2: a corr (tertial Literature 45.10	× C _d -(H) ₂) + (2 ary)) e - Calculated = 37.16 129.36 4.76 182.08	= Residual	Reference 37DOL/GRE	$\Delta_t G^\circ = \ln K_t = \frac{1 - \text{Butyne}}{1 \times C - (\text{I})}$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \frac{1 - \text{Butyne}}{1 \times C - (\text{I})}$	H)), σ = 3 Literatur	195.85 - 79.00 × C-(H) ₂ (C)(C e - Calculated 166.64 82.47 289.27	= Residual 1.41	C))+ Reference 51PRO/MAR
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	I) ₃ (C)) + (2: a corr (tertial Literature 45.10	× C _d -(H) ₂) + (2 ary)) e - Calculated = 37.16 129.36 4.76 182.08 255.14	= Residual	Reference 37DOL/GRE	$\Delta_t G^\circ = \ln K_t = \frac{1 \cdot \text{Butyne}}{1 \cdot \text{C} \cdot \text{C} \cdot \text{C}}$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \frac{1 \cdot \text{C}}{1 \cdot \text{C}}$	H)), σ = 3 Literatur 165.23 81.42	195.85 - 79.00 × C-(H) ₂ (C)(C e - Calculated 166.64 82.47 289.27 - 125.41	= Residual - 1.41 - 1.05	C))+ Reference 51PRO/MAR 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S_p^\circ = \Delta_t S^\circ =$	I) ₃ (C)) + (2: a corr (tertial Literature 45.10	× C _d -(H) ₂) + (2 ary)) e - Calculated = 37.16 129.36 4.76 182.08 255.14 -432.15	= Residual	Reference 37DOL/GRE	$\Delta_t G^\circ = \ln K_t = \frac{1 \cdot \text{Butyne}}{1 \cdot \text{C} \cdot \text{C} \cdot \text{C}}$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \frac{1 \cdot \text{C}}{1 \cdot \text{C}}$	H)), σ = 3 Literatur 165.23 81.42	195.85 - 79.00 × C-(H) ₂ (C)(C e - Calculated 166.64 82.47 289.27 - 125.41 204.03	= Residual - 1.41 - 1.05	C))+ Reference 51PRO/MAR 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	I) ₃ (C)) + (2: a corr (tertial Literature 45.10	× C _d -(H) ₂) + (2 ary)) e - Calculated = 37.16 129.36 4.76 182.08 255.14 -432.15 133.61	= Residual	Reference 37DOL/GRE	$\Delta_t G^\circ = \ln K_t = \frac{1 \cdot \text{Butyne}}{1 \cdot \text{C} \cdot \text{C} \cdot \text{C}}$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \frac{1 \cdot \text{C}}{1 \cdot \text{C}}$	H)), σ = 3 Literatur 165.23 81.42	195.85 - 79.00 × C-(H) ₂ (C)(C e - Calculated 166.64 82.47 289.27 - 125.41	= Residual - 1.41 - 1.05	Reference 51PRO/MAR 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	I) ₃ (C)) + (2: a corr (tertial Literature 45.10	× C _d -(H) ₂) + (2 ary)) e - Calculated = 37.16 129.36 4.76 182.08 255.14 -432.15	= Residual	Reference 37DOL/GRE	$\Delta_t G^\circ = \ln K_t = \frac{1 \cdot \text{Butyne}}{1 \cdot \text{C} \cdot \text{C} \cdot \text{C}}$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \frac{1 \cdot \text{C}}{1 \cdot \text{C}}$	H)), σ = 3 Literatur 165.23 81.42	195.85 - 79.00 × C-(H) ₂ (C)(C e - Calculated 166.64 82.47 289.27 - 125.41 204.03	= Residual - 1.41 - 1.05	Reference 51PRO/MAR 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	I) ₃ (C)) + (2: a corr (tertial Literature 45.10	× C _d -(H) ₂) + (2 ary)) e - Calculated = 37.16 129.36 4.76 182.08 255.14 -432.15 133.61	= Residual	Reference 37DOL/GRE	$\Delta_t G^\circ = \ln K_t = \frac{1 - \text{Butyne}}{1 \times \text{C} - (\text{F})}$ Gas Phase $\Delta_t H^\circ = C^\circ_t = S^\circ = \Delta_t S^\circ = 1 \ln K_t = \frac{1 \times \text{C}}{1 \times \text{C}}$	H)), σ = 3 Literatur 165.23 81.42	195.85 - 79.00 × C-(H) ₂ (C)(C e - Calculated 166.64 82.47 289.27 - 125.41 204.03	= Residual - 1.41 - 1.05	Reference 51PRO/MAR 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	I) ₃ (C)) + (2: a corr (tertial Literature 45.10	× C _d -(H) ₂) + (2 ary)) e - Calculated = 37.16 129.36 4.76 182.08 255.14 -432.15 133.61	= Residual	Reference 37DOL/GRE	$\Delta_t G^\circ = \ln K_t = \frac{1 - \text{Butyne}}{1 \times \text{C} - (\text{H})}$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1 - \text{Pentyne}}{1 \times \text{C} - (\text{H})}$	165.23 81.42 290.83	195.85 - 79.00 × C-(H) ₂ (C)(C) e - Calculated 166.64 82.47 289.27 - 125.41 204.03 - 82.30 × C-(H) ₂ (C) ₂)	= Residual - 1.41 - 1.05 1.56	C))+ Reference 51PRO/MAR 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	I) ₃ (C)) + (2: a corr (tertial Literature 45.10	× C _d -(H) ₂) + (2 ary)) e - Calculated = 37.16 129.36 4.76 182.08 255.14 -432.15 133.61	= Residual	Reference 37DOL/GRE	$\Delta_t G^\circ = \ln K_t = \frac{1 - \text{Butyne}}{1 \times \text{C} - (\text{H})}$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1 - \text{Pentyne}}{1 \times \text{C} - (\text{H})}$	165.23 81.42 290.83 H) ₃ (C)) + (1:C)) + (1 × C ₁	195.85 - 79.00 × C-(H) ₂ (C)(C) e - Calculated 166.64 82.47 289.27 - 125.41 204.03 - 82.30	= Residual - 1.41 - 1.05 1.56 + (1 × C-(H) ₂ (C))+ Reference 51PRO/MAR 69STU/WES 69STU/WES

TABLE 9. Alkynes (28) - Continued

TABLE 9. Alkynes (28) - Continued

$ \begin{array}{c} C_{\rm g}^{\circ} = & 162.84 \\ S^{\circ} = & 229.86 \\ A_{\rm h}S^{\circ} = & -321.12 \\ A_{\rm h}G^{\circ} = & 211.89 \\ InK_{\rm f} = & -85.48 \\ \end{array} $		$()_3(C)) + (1)$	\times C-(H) ₂ (C) ₂) -(H)), $\sigma = 3$	+ (1 × C-(H) ₂	C_5H_8 $(C)(C_1)) +$			$\times C-(H)_2(C)_2$ $(\tau-(H)), \sigma = 3$	+ (1 × C-(H) ₂	C ₈ H ₁₄ (C)(C ₁))+
		Literatur	e - Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
$ \begin{array}{c} C_c^* = & 162.84 \\ S^* = & 229.86 \\ S^* = & 229.86 \\ S^* = & -231.12 \\ A_G^* = & -211.189 \\ A_G^* = & -237.37 \\ A_G^* = & -237.30 \\ A_G$	Liquid Phas	e				Gas Phase				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\Delta_{\mathbf{f}}H^{\circ} =$		116.15				80.71	84.12	-3.41	79ROG/DAG
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C_{p}^{\circ} =$		162.84				173.97		- 0.06	69STU/WES
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			229.86			-	446.64		0.73	69STU/WES
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$										
Liquid Phase Liq			211.89							
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	$lnK_f =$, ,	- 85.48 			$lnK_f =$	· · · · · · · · · · · · · · · · · · ·	- 95.75		· · · · · · · · · · · · · · · · · · ·
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $						I iouid Pha	se.			
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1.Havuna				C.H.			38.96		
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		D-(C)) + (5	x ር-(ዘ)ኅርን-ን	+ (1 × C-(H)-						
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$. (17.0 (11)2	(-)(-))					
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	(1.7.4)	-,, . (1 ^)	()), 0 = 3							
InK _f = -91.84 InK _f = -91.91 InK _f = -91.84 InK _f = -91.91 InK _f = -91.84 InK _f = -91.91 InK _f = -91.91 InK _f = -91.84 InK _f = -91.91 InK _f = -91.91 InK _f = -91.91 InK _f = -91.84 InK _f = -91.91 InK _f = -91.91 InK _f = -91.84 InK _f = -91.91 InK _f = -91.84 InK _f = -91.91 InK _f = -91.91 InK _f = -91.84 InK _f = -91.91 InK _f =		Literatur	e - Calculated	= Residual	Reference					
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$						-				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$										
$\begin{array}{cccccccccccccccccccccccccccccccccccc$										
								· ·		C9H16
	s° =	368.74		1.15	69STU/WES				$+ (1 \times C - (H)_2)$	(C)(G))+
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$						(1×C _t -(0	$C))+(1\times C)$	$(-(H)), \sigma = 3$		
Liquid Phase $\Delta_t H^o = 90.42$ $\Delta_t H^o = 62.25$ 63.49 -1.24 $79ROG/DA$ $C_s^o = 193.26$ $C_s^o = 196.82$ 196.92 -0.10 $69STU/WES$ $S^o = 262.24$ $S^o = 485.60$ 485.07 0.53 $69STU/WES$ $\Delta_t G^o = 217.15$ $\Delta_t G^o = 245.71$ $\ln K_t = -87.60$ $\ln K_t = -99.12$ $\Delta_t H^o = 13.23$ $\Delta_t G^o = 245.71$ $\ln K_t = -99.12$ $\Delta_t H^o = 13.23$ $\Delta_t G^o = 39.36$ $\Delta_t G^o = 3$										
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\ln K_{\rm f} =$		- 89.03		·		Literatu	re – Calculated	= Residual	Reference
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Liquid Pho					Gas Phase				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	•	se	00.42				62.25	63.40	_124	70P.OG/DAG
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	-					-				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$								_		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$							405.00		0.55	09310/WL3
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$										
1-Heptyne $(1 \times C_{-}(H)_{3}(C)) + (3 \times C_{-}(H)_{2}(C)_{2}) + (1 \times C_{-}(H)_{2}(C)(C_{1})) + C_{-}(H)_{2}(C)(C_{1}) + $	-									
1-Heptyne $(1 \times C_{-}(H)_{3}(C)) + (3 \times C_{-}(H)_{2}(C)_{2}) + (1 \times C_{-}(H)_{2}(C)(C_{1}) + C_{-}(C_{1}) + C$										· · · · · · · · · · · · · · · · · · ·
$\begin{array}{cccccccccccccccccccccccccccccccccccc$							se			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		T) (C)) . (2		1 (1 × C (T)						
Literature - Calculated = Residual Reference				+ (1 × C-(H)2	(C)(G))+					
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	(1×C-(0	J))+(1×C	$-(H)$, $\sigma = 3$							
Gas Phase $\Delta_{l}H^{\circ} = 103.76 104.75 -0.99 79\text{ROG/DAG}$ $C_{p}^{\circ} = 151.08 151.14 -0.06 69\text{STU/WES}$ $S^{\circ} = 407.69 406.75 0.94 69\text{STU/WES}$ $\Delta_{l}G^{\circ} = 229.04 101.16 -92.39$ Liquid Phase $\Delta_{l}H^{\circ} = 64.69 \Delta_{l}H^{\circ} = 41.88 42.86 -0.98 79\text{ROG/DAG}$ $C_{p}^{\circ} = 229.64 C_{p}^{\circ} = 223.68 C_{p}^{\circ} = 219.70 219.81 -0.11 69\text{STU/WES}$ $S^{\circ} = 294.62 S^{\circ} = 524.51 524.23 0.28 69\text{STU/WES}$ $\Delta_{l}G^{\circ} = 222.41 \Delta_{l}G^{\circ} = 254.04$		7 14		Destained	D - f					
Gas Phase $\Delta_t H^\circ = 103.76 104.75 -0.99 79 \text{ROG/DAG}$ $C_p^\circ = 151.08 151.14 -0.06 69 \text{STU/WES}$ $S^\circ = 407.69 406.75 0.94 69 \text{STU/WES}$ $\Delta_t S^\circ = -416.86$ $\Delta_t G^\circ = 229.04$ $\ln K_t = -92.39$ Liquid Phase $\Delta_t H^\circ = 64.69$ $C_p^\circ = 223.68$ $S^\circ = 294.62$ $\Delta_t S^\circ = -528.99$ $\Delta_t G^\circ = 222.41$ $\Delta_t S^\circ = -708.31$ $\Delta_t G^\circ = 222.41$		Literatur	e - Calculated	= Kesiduai	Reference					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$.,						75.70		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$										
$\begin{array}{cccccccccccccccccccccccccccccccccccc$										
$\begin{array}{cccccccccccccccccccccccccccccccccccc$							r) (~')			C10H18
$\Delta_t G^\circ = 229.04 \ lnK_t = -92.39$ Literature - Calculated = Residual Reference Liquid Phase $\Delta_t H^\circ = 64.69$ $C_p^\circ = 223.68$ $C_p^\circ = 223.68$ $C_p^\circ = 294.62$ $C_p^\circ = 524.51$ $C_p^\circ = 524.23$ $C_p^\circ = 524.51$ $C_p^\circ = 69.51$ C	-	407.69		0.94	69STU/WES				$+(1\times C-(H)_2)$	(C)(C _i))+
Liquid Phase Gas Phase $\Delta_t H^\circ =$ 64.69 $\Delta_t H^\circ =$ 41.88 42.86 -0.98 79ROG/DAG $C_p^\circ =$ 223.68 $C_p^\circ =$ 219.70 219.81 -0.11 69STU/WES $S^\circ =$ 294.62 $S^\circ =$ 524.51 524.23 0.28 69STU/WES $\Delta_t S^\circ =$ -528.99 $\Delta_t S^\circ =$ -708.31 $\Delta_t G^\circ =$ 222.41 $\Delta_t G^\circ =$ 254.04						(1×C₁-(0	ر(ر))+(1×C	$\sigma(H)$, $\sigma=3$		
Liquid Phase $ \Delta_t H^\circ = \qquad $							T :		D	D. C
$\Delta_t H^\circ = 64.69$ $\Delta_t H^\circ = 41.88$ 42.86 -0.98 $79ROG/DAG$ $C_\rho^\circ = 223.68$ $C_\rho^\circ = 219.70$ 219.81 -0.11 $69STU/WES$ $S^\circ = 294.62$ $S^\circ = 524.51$ 524.23 0.28 $69STU/WES$ $\Delta_t S^\circ = -708.31$ $\Delta_t G^\circ = 222.41$ $\Delta_t G^\circ = 254.04$	$lnK_f =$		- 92.39				Literatui	e – Calculated	= Residual	Reference
$\Delta_t H^\circ = 64.69$ $\Delta_t H^\circ = 41.88$ 42.86 -0.98 $79ROG/DAG$ $C_p^\circ = 223.68$ $C_p^\circ = 219.70$ 219.81 -0.11 $69STU/WES$ $S^\circ = 294.62$ $S^\circ = 524.51$ 524.23 0.28 $69STU/WES$ $\Delta_t S^\circ = -708.31$ $\Delta_t G^\circ = 222.41$ $\Delta_t G^\circ = 254.04$	Liquid Pho	se				Gas Phase				
$C_p^{\circ} =$ 223.68 $C_p^{\circ} =$ 219.70 219.81 -0.11 69STU/WES $S^{\circ} =$ 294.62 $S^{\circ} =$ 524.51 524.23 0.28 69STU/WES $\Delta_t S^{\circ} =$ -528.99 $\Delta_t S^{\circ} =$ -708.31 $\Delta_t G^{\circ} =$ 222.41 $\Delta_t G^{\circ} =$ 254.04			64 69				41.88	42.86	_0.98	79ROG/DAG
$S^{\circ} = 294.62$ $S^{\circ} = 524.51$ 524.23 0.28 69STU/WES $\Delta_{c}S^{\circ} = -528.99$ $\Delta_{c}S^{\circ} = -708.31$ $\Delta_{c}G^{\circ} = 222.41$ $\Delta_{c}G^{\circ} = 254.04$	-									
$\Delta_{r}S^{\circ} = -528.99$ $\Delta_{f}S^{\circ} = -708.31$ $\Delta_{f}G^{\circ} = 222.41$ $\Delta_{f}G^{\circ} = 254.04$	•									
$\Delta_t G^\circ = 222.41 \qquad \Delta_t G^\circ = 254.04$						Δ.S° =	J27,J1		0.20	09910/WE9
The state of the s						-				
						1				

TABLE 9. Alkynes (28) - Continued

TABLE	9.	Alkynes	(28)	_	Continued
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(1×G-(C)	₃ (C))+(6×))+(1×C ₁ -	$C-(H)_2(C)_2$ (H)), $\sigma = 3$	+ (1 × C-(H) ₂ ($C_{10}H_{18}$ $C(C_1) +$	(2×0-(1.	I)₃(C))+(2	× C ₁ -(C)), σ =	= 18	C4
		- Calculated	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
					Liquid Phas	se			
Gas Phase					$\Delta_t H^\circ =$	118.53	119.08	-0.55	50AST/MAS
	44.00	40.06	0.00	70D O O D A C					
$\Lambda_i H^{\circ} =$	41.88	42.86	-0.98	79ROG/DAG	$C_{\rho}^{\circ} =$	124.14	124.14	0.00	50AST/MAS
$C_{P}^{\circ} =$	219.70	219.81	-0.11	69STU/WES	S° =	195.10	195.10	0.00	50AST/MAS
<i>S</i> ° =	524.51	524.23	0.28	69STU/WES	$\Delta_f S^\circ =$		-219.57		
$\Delta_f S^\circ =$		-708.31			$\Delta_{\mathbf{f}}G^{\circ} =$		184.55		
$\Delta_{\rm f}G^{\circ} =$		254.04		W.	$lnK_f =$		- 74.44		
$lnK_f =$		-102.48			-				
iquid Phase					2-Pentyne				C _s
	5	- 12.50				D (C)\ . (1	v.C. (II) (C)(C		
$A_iH^\circ =$					(2×C-(F	1/3(U)/+(1	\times C-(H) ₂ (C)(C	<i>111</i> + (4 × 4 − (1	$\cup_{IJ}, \sigma = y$
$C_p^o =$		314.94				T :4		D!!	D.C.
<i>S</i> ° =		391.76				Literatur	e – Calculated	= Kesidual	Reference
Δ _ι ς° =		- 840.78							
$_iG^{\circ} =$		238.18							
$\ln K_{\rm f} =$		- 96.08			Gas Phase				
					$\Delta_{\rm f}H^{\circ} =$	128.87	125.98	2.89	69STU/WES
				THE RESERVE TO SERVE THE PERSON OF THE PERSO	$C_p^{\circ} =$	98.70	98.87	- 0.17	69STU/WES
					S° =	331.79	331.81	-0.02	69STU/WES
-Hexadecyn				C ₁₆ H ₃₀	$\Delta_{\mathfrak{t}}S^{\circ} =$		-219.17		
		\times C-(H) ₂ (C) ₂)+(1×C-(H)	₂(C)(C₁))+	$\Delta_{\rm f}G^{\circ} =$		191.33		
(1 × C _i -(C	$(1 \times C_t$	$-(H)), \sigma = 3$			$lnK_f =$		<i>−77.</i> 18		
•	Literature	- Calculated	= Residual	Reference					
					Liquid Phas	se	06.05		
					$\Delta_t H^\circ =$		96.95		
as Phase					$C_p^{\circ} =$		154.53		
$\Delta_i H^\circ =$		-80.92			<i>S</i> ° =		227.46		
$C_p^{\circ} =$	356.94	357.15	-0.21	69STU/WES	$\Delta_f S^\circ =$		-323.52		
S° =	758.22	759.19	-0.97	69STU/WES	$\Delta_t G^{\circ} =$		193.41		
$\Delta_f S^\circ =$	100.22	- 1291.22	5.77	0,010/1120	$\ln K_{\rm f} =$		-78.02		
					nnzt –		70.02		
$\Delta_t G^\circ = \ln K_t =$		304.06 122.65							······································
-					3-Methyl-1-	butvne			Csl
Liquid Phas	e				•	•	× C-(H)(C) ₂ (C	Z))+	
$\Delta_t H^\circ =$	-	166.88					(11)(2)(2) ary)) + $(1 \times C_1$		$(H)), \sigma = 0$
$C_p^{\circ} =$		497.46			(011)	, ((-)) . (1)	()),
						T :+	o Colout-4-3	m Docidu-1	Dofores
S° =		586.04				Literatur	e – Calculated	– Residuai	Reference
4 00		- 1464.36							
		269.72							
$\Delta_i G^\circ =$									
$\Delta_t G^{\circ} =$		108.80			Gas Phase				
$\Delta_t G^{\circ} =$						136,40	136.40	0.00	69STU/WES
					$\Delta_f H^\circ =$			0.00	
					$\Delta_{\rm f}H^{\circ} = C_{\rm P}^{\circ} =$	104.68	104.68	0.00	69STU/WES
$\Delta_f G^\circ = \ln K_f =$				CH	$\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} =$		104.68 318.96		
$\Delta_f G^\circ = \ln K_f =$ -Butyne	0 (0) 1 (2)	108.80	10	C ₄ H ₆	$\Delta_{\mathbf{f}}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{\mathbf{f}}S^{\circ} =$	104.68	104.68 318.96 -232.02	0.00	69STU/WES
$\Delta_f G^\circ = \ln K_f = \frac{1}{2}$	() ₃ (C))+(2:		= 18	C ₄ H ₆	$\Delta_t H^\circ = C_P^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	104.68	104.68 318.96 -232.02 205.58	0.00	69STU/WES
$\Delta_f G^\circ = \ln K_f = \frac{1}{2}$		108.80 < C ₁ -(C)), σ =			$\Delta_{\mathbf{f}}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{\mathbf{f}}S^{\circ} =$	104.68	104.68 318.96 -232.02	0.00	69STU/WES
$\Delta_f G^\circ = \ln K_f =$ -Butyne		108.80		C₄H ₆	$\Delta_t H^\circ = C_P^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	104.68	104.68 318.96 -232.02 205.58	0.00	69STU/WES
$\Delta_f G^\circ = InK_f = In$		108.80 < C ₁ -(C)), σ =			$\Delta_t H^\circ = C_P^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	104.68	104.68 318.96 -232.02 205.58	0.00	69STU/WES
$\Delta_t G^\circ = InK_t = InK_t = InK_t$ -Butyne (2 × C-(H	Literature	108.80 < C _t (C)), σ = e Calculated	= Residual	Reference	$\Delta_t H^\circ = C_P^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	104.68	104.68 318.96 -232.02 205.58	0.00	69STU/WES
$\Delta_t G^\circ = \ln K_t = $ -Butyne $(2 \times C - (H + Gas Phase \Delta_t H^\circ = Gas Phase D_t H^\circ = G$	Literature	108.80 < C ₁ (C)), σ = e Calculated 145.68	= Residual - 0.54	Reference 51PRO/MAR	$\Delta_t H^\circ = C_P^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	104.68	104.68 318.96 -232.02 205.58	0.00	69STU/WES
$\Delta_t G^\circ = \ln K_t = \frac{1}{2}$ Butyne $(2 \times C - (H + G^\circ))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = \frac{1}{2}$	Literature 145.14 77.95	108.80 < C ₁ -(C)), σ = e - Calculated 145.68 77.90	= Residual - 0.54 0.05	Reference 51PRO/MAR 69STU/WES	$\Delta_t H^\circ = C_P^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	104.68	104.68 318.96 -232.02 205.58	0.00	69STU/WES
$\Delta_t G^\circ = \ln K_t = $ 3-Butyne $(2 \times C - (H + G^\circ))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = $	Literature	108.80 < C ₁ (C)), σ = e Calculated 145.68	= Residual - 0.54	Reference 51PRO/MAR	$\Delta_t H^\circ = C_P^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	104.68	104.68 318.96 -232.02 205.58	0.00	69STU/WES
$\Delta_f G^\circ = InK_f = In$	Literature 145.14 77.95	108.80 < C ₁ -(C)), σ = e - Calculated 145.68 77.90	= Residual - 0.54 0.05	Reference 51PRO/MAR 69STU/WES	$\Delta_t H^\circ = C_P^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	104.68	104.68 318.96 -232.02 205.58	0.00	69STU/WES
$\Delta_t G^\circ = InK_t = In$	Literature 145.14 77.95	108.80 < C ₁ -(C)), σ = e - Calculated 145.68 77.90 283.25	= Residual - 0.54 0.05	Reference 51PRO/MAR 69STU/WES	$\Delta_t H^\circ = C_P^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	104.68	104.68 318.96 -232.02 205.58	0.00	69STU/WES

TABLE 9.	Alkynes	(28) $-$	Continued
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TABLE 9. Alkynes (28) - Continued

	$(H)_1 + (1 \times C_1)_2, \ \sigma = 2$	$-(C_d)$) + (1 × C_d	<u>-</u> (H)(C₁))+				\times C-(H) ₂ (C) ₂) \times C _d -(H)(C ₁))		$(C)(C_d)$) +) + (1 × C_t –(H))
	Literature	e – Calculated =	Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	73.18 279.37	289.52 73.18 279.38	0.00 -0.01	69STU/WES 69STU/WES	Gas Phase $\Delta_t H^\circ = C_p^\circ =$		153.86 208.46		
$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$		-4.73 290.93 -117.36			Liquid Phas $\Delta_t H^\circ =$	se 100.75	96,21	4.54	59SKI/SNE
cis-3-Pente (1 × C-(1	H)₃(C))+(1× + (1×C₁−	$(H)) + (1 \times cis)$	unsat) corr)	C_5H_6 $(C_1) + (1 \times C_1 - (C_d))$		$(C) + (2 \times C) + (2 \times C)$	× C-(H) ₂ (C) ₂) -(C _d))+(1 × C	C_{d} -(H)(C_{i})) + ($1 \times C_{d}$ $-(H)_2)$
	Literatur	e – Calculated =	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas Phase $\Delta_t H^\circ = C_p^\circ =$		262.11 88.24			Gas Phase $\Delta_t H^\circ = C_p^\circ =$		187.90 156.33		
Liquid Pha Δ _ε H° =	226.35	230.13	-3.78	59SKI/SNE	Liquid Phas $\Delta_t H^\circ =$	se 140.71	144.65	-3.94	57FLI/SKI
trans -3-Per (1 × C–(1	H) ₃ (C))+(1		(1×C _d −(H)(C_5H_6 $C_1) + (1 \times C_1 - (C_d))$	Butadiyne (2×C ₁ –(F	·I))+(2×C ₁	$(-(C_t)), \sigma = 2$		C ₄ F
	+ (1×C ₁ -	(H)) e – Calculated =	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
					Gas Phase $\Delta_t H^\circ =$	472.79 73.64	468.52 73.64	4.27 0.00	69STU/WES
Gas Phase $\Delta_t H^\circ = C_p^\circ =$ Liquid Pha		257.26 96.27	·		$C_{\rho}^{\circ} = S^{\circ} = S_{f}S^{\circ} = \Delta_{f}S^{\circ} = \ln K_{f} = 0$	250.04	250.04 96.51 439.75 - 177.39	0.00	69STU/WES 69STU/WES
$\Delta_t H^\circ = C_p^\circ =$			3.16	59SKI/SNE	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = 0$		250.04 96.51 439.75		
$\Delta_{\ell}H^{\circ} = C_{p}^{\circ} = $ Liquid Pha $\Delta_{\ell}H^{\circ} = $ cis-3-Decen	ase 228.02	96.27		C ₁₀ H ₁₆	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = \frac{1,5\text{-Hexadiy}}{1}$	250.04 ne	250.04 96.51 439.75	0.00	
$\Delta_t H^\circ = C_p^\circ =$ Liquid Pha $\Delta_t H^\circ =$ $(1 \times C_t - (1 \times C_t - 1))$	ase 228.02 n-1-yne H) ₃ (C)) + (4	96.27 224.86 × C-(H) ₂ (C) ₂)- × cis (unsat) cor	+ (1 × C–(H) ₂ ($C_{10}H_{16}$ (C)(C _d)) +	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = \frac{1,5\text{-Hexadiy}}{1}$	250.04 ne H)) + (2 × C _t	250.04 96.51 439.75 -177.39	0.00 -(H) ₂ (C ₁) ₂)	69STU/WES
$\Delta_t H^\circ = C_p^\circ =$ Liquid Pha $\Delta_t H^\circ =$ $(1 \times C_t - (1 \times C_t - 1))$	n-1-yne H) ₃ (C)) + (4 (H)(C)) + (1 (C _d)) + (1 × C	96.27 224.86 × C-(H) ₂ (C) ₂)- × cis (unsat) cor	+ (1 × C–(H) ₂ / rr) + (1 × C _d –($C_{10}H_{16}$ (C)(C _d)) +	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = \frac{1,5\text{-Hexadiy}}{1}$	250.04 ne H)) + (2 × C _t	250.04 96.51 439.75 -177.39	0.00 -(H) ₂ (C ₁) ₂)	69STU/WES

TARTE O	Allamos	(28)	Continued
I ABLE 9.	Aikvnes	(28) —	Continuea

TABLE 9. Alkynes (28) - Continued

1,7-Octadiy (2×C₁-(1		-(C))+(2×C-	$(H)_2(C)(C_1))$	$C_8H_{10} + (2 \times C - (H)_2(C)_2)$		3(C))+(1)		< C₁−(C)) + (1	C_6H_{16} × C-(C) ₃ (C ₁)) +
	Literature	- Calculated =	= Residual	Reference	(3×−CH ₃	`.	ernary)) ture-Calculated	1 — Dosidual	Reference
						Litera	ure-Calculated	i = Kesiduai	Reference
Gas Phase $\Delta_t H^\circ = C_p^\circ =$		376.54 159.26			Liquid Phase Δ _f H° =	78.45	78.45	0.00	77KUP/SHI
Liquid Pha $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} =$	se 334.72	327.52 252.72 293.12	7.20	57FLI/SKI	3,3-Dimethyl (2×C-(H)		liyne < C _t -(H)) + (2 >	< C _i -(C))+(1	C_7H_1 × C-(C) ₂ (C ₁) ₂)
$\Delta_f S^\circ = \Delta_f G^\circ =$		-405.65 448.47				Litera	ure-Calculated	l = Residual	Reference
$lnK_f =$		- 180.91			Liquid Phase $\Delta_t H^\circ =$	348.69	348.69	0.00	77KUP/SHI
3,9-Dodeca (2 × C-(I (2 × C-(I	H) ₃ (C))+(4> H) ₂ (C) ₂)	< C-(H)₂(C)(C e – Calculated =		C ₁₂ H ₁₈ C)) + Reference		3(C))+(2> 3(C ₁))+(4>		uaternary))	$C_{12}H_{11}$ + $(2 \times C_1 - (C))$ +
Gas Phase									
$\Delta_{f}H^{\circ} = C_{p}^{\circ} = -$		255.82 234.00			Liquid Phase $\Delta_t H^\circ =$	211.08	209.44	1.64	77KUP/SHI
Liquid Pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	se 196.61	193.40 357.72 417.80 -826.22	3.21	57FLI/SKI	2,2,7,7-Tetrar (6×C-(H) (6×-CH ₃ (3(C))+(2>	$(C-(C)_3(C_1))+$	· (2×C,-(C)) +	C12H16 +(2×C1-(C1))+
$\Delta_l G^\circ = \ln K_l =$		439.74 177.39				Literat	ure-Calculated	l = Residual	Reference
	H)3(C))+(4)	< C-(H) ₂ (C) ₂) -	+ (2×C-(H) ₂	$C_{12}H_{18}$ $(C)(C_1)) +$	Liquid Phase $\Delta_t H^\circ =$		157.56		
(2×G-(C))+(2×C _t - Literature	=(G)) = – Calculated =	= Residual	Reference	Solid Phase $\Delta_t H^\circ =$	156.10	156.10	0.00	77KUP/SHI
Gas Phase									
$\Delta_i H^\circ = C_p^\circ =$		265.28 239.94							

TABLE 10. Aromatic CH-01 (42)

Benzene (6×C _B -(H)(C _B) ₂), σ	= 12		C ₆ H ₆	1,2-Dimethy (2×C-(F		$\times C_B - (H)(C_B)$	2)+(2×C _B -(C	C_8H_1
(2 (, , , ,					corr), σ =			
	Literatur	e – Calculated —————	= Residual	Reference		Literatur	re – Calculated	= Residual	Reference
Gas phase								· · · · · · · · · · · · · · · · · · ·	
$\Delta_i H^{\circ} =$	82.80	82.86	-0.06	47OSB/GIN	Gas phase				
$C_p^{\circ} =$	81.67	81.66	0.01	69STU/WES	$\Delta_{\mathbf{f}}H^{\circ} =$	19.08	19.26	-0.18	47OSB/GIN
S° =	269.20	269.20	0.00	69STU/WES	$C_p^{\circ} =$	133.26	131.80	1.46	69STU/WES
$\Delta_{\mathbf{f}}S^{\circ} =$		- 156.95			. S° =	352.75	350.13	2.62	69STU/WES
$\Delta_{\rm f}G^{\circ} =$		129.66			$\Delta_f S^\circ =$		-348.65		
$\ln K_{\rm f} =$		-52.30			$\Delta_{\rm r}G^{\circ} =$		123.21		
					$lnK_f =$		-49.70		
Liquid phas	se								
$\Delta_t H^\circ =$	48.95	48.96	-0.01	69GOO/SMI	Liquid phas	se			
$C_p^{\circ} =$	136.06	136.08	-0.02	48OLI/EAT	$\Delta_{\mathbf{f}}H^{\circ} =$	-24.35	~21.00	- 3.35	45PRO/GIL
S° =	173.26	173.22	0.04	48OLI/EAT	$C_p^{\circ} =$	187.82	187.38	0.44	43PIT/SCO
$\Delta_{\mathbf{f}}S^{\circ} =$		-252.93			S° =	246.02	243.08	2.94	43PIT/SCO
$\Delta_t G^{\circ} =$		124.37			$\Delta_{\mathbf{f}}S^{\circ} =$		- 455.69		
$\ln K_{\rm f} =$		-50.17			$\Delta_{\mathbf{f}}G^{\circ} =$		114.87		
					$lnK_f =$		-46.34		
Solid phase	;								· <u>·</u>
$\Delta_{f}H^{\circ} =$	39.08	39.18	-0.10	48OLI/EAT					
$C_p^{\circ} =$		120.78			1,3-Dimethy				C ₈ H ₁
S° =		136.50			(2×C-(H	I)₃(C))+(4	$\times C_B - (H)(C_B)_2$	$(2 \times C_B - (C$	$C)(C_B)_2) +$
$\Delta_f S^\circ =$		-289.65			(1×meta	corr), $\sigma =$	18		
$\Delta_f G^\circ =$		125.54							
						T itamatum	e - Calculated	- Pacidual	Reference
$lnK_f =$		- 50.64				Literatur			
Toluene	, , ,, ,			C_7H_8 $C_7(C_D)_2$, $\sigma = 6$ Reference	Gas phase $\Delta_t H^\circ = C_r^\circ = S^\circ = \Delta_t S^\circ =$	17.32 127.57 357.69	17.37 126.11 352.63 - 346.15	- 0.05 1.46 5.06	47OSB/GIN 69STU/WES 69STU/WES
Toluene	, , ,, ,	× C _B (H)(C _B) ₂		$C)(C_{\rm B})_2), \sigma = 6$	$\Delta_l H^{\circ} = C_p^{\circ} = S^{\circ} =$	17.32 127.57	17.37 126.11 352.63	-0.05 1.46	47OSB/GIN 69STU/WES
Toluene	, , ,, ,	× C _B (H)(C _B) ₂		$C)(C_{\rm B})_2), \sigma = 6$	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = S^{\circ} = S^{\circ}$	17.32 127.57	17.37 126.11 352.63 - 346.15 120.57	-0.05 1.46	47OSB/GIN 69STU/WES
Toluene (1 × C-(F	, , ,, ,	× C _B (H)(C _B) ₂		$C)(C_{\rm B})_2), \sigma = 6$	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = S^{\circ} = S^{\circ}$	17.32 127.57	17.37 126.11 352.63 - 346.15 120.57	-0.05 1.46	47OSB/GIN 69STU/WES
Toluene $(1 \times C - (I))$ Gas phase $\Delta_t H^\circ =$	Literatur	× C _n –(H)(C _n) ₂ e – Calculated	= Residual	$(C_D)_2$, $\sigma = 6$ Reference	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = S^{\circ} = S^{\circ}$	17.32 127.57 357.69	17.37 126.11 352.63 - 346.15 120.57	-0.05 1.46	47OSB/GIN 69STU/WES
Toluene (1×C-(I	Literatur	\times C _n -(H)(C _n) ₂ e - Calculated 50.43	= Residual	$(C_D)_2$, $\sigma = 6$ Reference 47OSB/GIN	$\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{\ell}S^{\circ} = \Delta_{\ell}G^{\circ} = \ln K_{\ell} = \frac{1}{2}$	17.32 127.57 357.69	17.37 126.11 352.63 - 346.15 120.57	-0.05 1.46	47OSB/GIN 69STU/WES
Toluene $(1 \times C - (I))$ Gas phase $\Delta_t H^\circ = C_p^\circ =$	50.00 103.64	× C _n -(H)(C _n) ₂ e - Calculated 50.43 103.53	= Residual - 0.43 0.11	$(C_D)_2$, $\sigma = 6$ Reference 47OSB/GIN 69STU/WES	$\Delta_t H^\circ = C_r^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phas $\Delta_t H^\circ = S^\circ = \Delta_t H^\circ = S^\circ = \Delta_t H^\circ = S^\circ = S^\circ = \Delta_t H^\circ = S^\circ $	17.32 127.57 357.69	17.37 126.11 352.63 - 346.15 120.57 - 48.64	-0.05 1.46 5.06	47OSB/GIN 69STU/WES 69STU/WES
Toluene $(1 \times C - (I \times C - (I \times C - (I \times C + ($	50.00 103.64	× C _p -(H)(C _p) ₂ e - Calculated 50.43 103.53 318.36	= Residual - 0.43 0.11	$(C_D)_2$, $\sigma = 6$ Reference 47OSB/GIN 69STU/WES	$\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{\ell}S^{\circ} = \Delta_{\ell}G^{\circ} = \ln K_{\ell} = $ Liquid phas	17.32 127.57 357.69	17.37 126.11 352.63 -346.15 120.57 -48.64	- 0.05 1.46 5.06 - 1.10 - 0.70	47OSB/GIN 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO
Toluene $(1 \times C - (I \times C - (I \times C - (I \times C + ($	50.00 103.64	× C _p -(H)(C _p) ₂ e - Calculated 50.43 103.53 318.36 - 244.10 123.21	= Residual - 0.43 0.11	$(C_D)_2$, $\sigma = 6$ Reference 47OSB/GIN 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid phas $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \frac{1}{2}$	17.32 127.57 357.69	17.37 126.11 352.63 -346.15 120.57 -48.64 -24.26 183.88 243.08	-0.05 1.46 5.06	47OSB/GIN 69STU/WES 69STU/WES
Toluene $(1 \times C - (I \times C - (I \times C - (I \times C + ($	50.00 103.64	× C _n -(H)(C _n) ₂ e - Calculated 50.43 103.53 318.36 - 244.10	= Residual - 0.43 0.11	$(C_D)_2$, $\sigma = 6$ Reference 47OSB/GIN 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid phas $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \frac{1}{2}$	17.32 127.57 357.69	17.37 126.11 352.63 -346.15 120.57 -48.64 -24.26 183.88 243.08 -455.69 111.61	- 0.05 1.46 5.06 - 1.10 - 0.70	47OSB/GIN 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO
Toluene $(1 \times C - (I))$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 1$ Liquid pha	50.00 103.64 320.66	× C _n -(H)(C _n) ₂ e - Calculated 50.43 103.53 318.36 - 244.10 123.21 - 49.70	= Residual - 0.43 0.11 2.30	Reference 47OSB/GIN 69STU/WES 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid phas $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \frac{1}{2}$	17.32 127.57 357.69	17.37 126.11 352.63 - 346.15 120.57 - 48.64 - 24.26 183.88 243.08 - 455.69	- 0.05 1.46 5.06 - 1.10 - 0.70	47OSB/GIN 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO
Toluene $(1 \times C - (I \times C))))))))))))))))))$	50.00 103.64 320.66	× C _p -(H)(C _p) ₂ e - Calculated 50.43 103.53 318.36 - 244.10 123.21	= Residual - 0.43 0.11	$(C_D)_2$, $\sigma = 6$ Reference 47OSB/GIN 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid phas $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \frac{1}{2}$	17.32 127.57 357.69	17.37 126.11 352.63 -346.15 120.57 -48.64 -24.26 183.88 243.08 -455.69 111.61	- 0.05 1.46 5.06 - 1.10 - 0.70	47OSB/GIN 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO
Toluene $(1 \times C - (I))$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 1$ Liquid pha	50.00 103.64 320.66	× C _n -(H)(C _n) ₂ e - Calculated 50.43 103.53 318.36 - 244.10 123.21 - 49.70	= Residual - 0.43 0.11 2.30	Reference 47OSB/GIN 69STU/WES 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid phas $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \frac{1}{2}$	17.32 127.57 357.69	17.37 126.11 352.63 -346.15 120.57 -48.64 -24.26 183.88 243.08 -455.69 111.61	- 0.05 1.46 5.06 - 1.10 - 0.70	47OSB/GIN 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO 43PIT/SCO
Toluene $(1 \times C - (I \times C)))))))))))))))))))))$	50.00 103.64 320.66	SO.43 103.53 318.36 - 244.10 123.21 - 49.70	- 0.43 0.11 2.30	P(C _D) ₂), σ = 6 Reference 47OSB/GIN 69STU/WES 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid phas $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \frac{1}{2}$	17.32 127.57 357.69 se -25.36 183.18 253.80	17.37 126.11 352.63 -346.15 120.57 -48.64 -24.26 183.88 243.08 -455.69 111.61	- 0.05 1.46 5.06 - 1.10 - 0.70	47OSB/GIN 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO 43PIT/SCO
Toluene $(1 \times C - (I \times C - (I \times C - (I \times C + (I$	50.00 103.64 320.66	S0.43 103.53 318.36 -244.10 123.21 -49.70	- 0.43 0.11 2.30 - 0.34 - 2.75	Reference 47OSB/GIN 69STU/WES 69STU/WES 69GOO/SMI 62SCO/GUT	$\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{1}{4}$ Liquid phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{1}{4}$ 1,4-Dimethy	17.32 127.57 357.69 se - 25.36 183.18 253.80	17.37 126.11 352.63 - 346.15 120.57 - 48.64 - 24.26 183.88 243.08 - 455.69 111.61 - 45.02	- 0.05 1.46 5.06 - 1.10 - 0.70 10.72	47OSB/GIN 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO 43PIT/SCO
Toluene $(1 \times C - (I \times C))))))))))))))))))$	50.00 103.64 320.66	50.43 103.53 318.36 - 244.10 123.21 - 49.70 12.35 159.98 208.15	- 0.43 0.11 2.30 - 0.34 - 2.75	Reference 47OSB/GIN 69STU/WES 69STU/WES 69GOO/SMI 62SCO/GUT	$\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{1}{4}$ Liquid phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{1}{4}$ 1,4-Dimethy	17.32 127.57 357.69 se - 25.36 183.18 253.80	17.37 126.11 352.63 - 346.15 120.57 - 48.64 - 24.26 183.88 243.08 - 455.69 111.61 - 45.02	- 0.05 1.46 5.06 - 1.10 - 0.70 10.72	47OSB/GIN 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO 43PIT/SCO
Toluene $(1 \times C - (I \times C)))))))))))))))))))))$	50.00 103.64 320.66	50.43 103.53 318.36 -244.10 123.21 -49.70 12.35 159.98 208.15 -354.31	- 0.43 0.11 2.30 - 0.34 - 2.75	Reference 47OSB/GIN 69STU/WES 69STU/WES 69GOO/SMI 62SCO/GUT	$\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{1}{4}$ Liquid phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{1}{4}$ 1,4-Dimethy	17.32 127.57 357.69 se - 25.36 183.18 253.80	17.37 126.11 352.63 - 346.15 120.57 - 48.64 - 24.26 183.88 243.08 - 455.69 111.61 - 45.02	-0.05 1.46 5.06 -1.10 -0.70 10.72	47OSB/GIN 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO 43PIT/SCO
Toluene $(1 \times C - (I \times C)))))))))))))))))))))$	50.00 103.64 320.66	50.43 103.53 318.36 -244.10 123.21 -49.70 12.35 159.98 208.15 -354.31 117.99	- 0.43 0.11 2.30 - 0.34 - 2.75	Reference 47OSB/GIN 69STU/WES 69STU/WES 69GOO/SMI 62SCO/GUT	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{C_{p}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1,4\text{-Dimethy}}{(2 \times \text{C-(F)})^{\circ}}$	17.32 127.57 357.69 se - 25.36 183.18 253.80	17.37 126.11 352.63 - 346.15 120.57 - 48.64 - 24.26 183.88 243.08 - 455.69 111.61 - 45.02 × C _B -(H)(C _B) ₂	-0.05 1.46 5.06 -1.10 -0.70 10.72	47OSB/GIN 69STU/WES 69STU/WES 4SPRO/GIL 43PIT/SCO 43PIT/SCO 43PIT/SCO
Toluene $(1 \times C - (I \times C)))))))))))))))))))))$	50.00 103.64 320.66	50.43 103.53 318.36 -244.10 123.21 -49.70 12.35 159.98 208.15 -354.31 117.99	- 0.43 0.11 2.30 - 0.34 - 2.75	Reference 47OSB/GIN 69STU/WES 69STU/WES 69GOO/SMI 62SCO/GUT	$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ 1,4-Dimethy (2 × C-(F)	17.32 127.57 357.69 se - 25.36 183.18 253.80 vlbenzene (I) ₃ (C)) + (4 Literatur	17.37 126.11 352.63 -346.15 120.57 -48.64 -24.26 183.88 243.08 -455.69 111.61 -45.02 × C _B -(H)(C _B) ₂	-0.05 1.46 5.06 -1.10 -0.70 10.72)+(2×C _B -(C	47OSB/GIN 69STU/WES 69STU/WES 4SPRO/GIL 43PIT/SCO 43PIT/SCO C ₈ H _H (C _B) ₂), σ = 18 Reference
Toluene $(1 \times C - (I \times C)))))))))))))))))))))$	50.00 103.64 320.66	50.43 103.53 318.36 -244.10 123.21 -49.70 12.35 159.98 208.15 -354.31 117.99	- 0.43 0.11 2.30 - 0.34 - 2.75	Reference 47OSB/GIN 69STU/WES 69STU/WES 69GOO/SMI 62SCO/GUT	$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = $ 1,4-Dimethy $(2 \times C - (H))$ Gas phase $\Delta_t H^\circ = (H)$	17.32 127.57 357.69 se -25.36 183.18 253.80 dbenzene (1) ₃ (C)) + (4 Literatur	17.37 126.11 352.63 -346.15 120.57 -48.64 -24.26 183.88 243.08 -455.69 111.61 -45.02 × C _B -(H)(C _B) ₂ c Calculated	-0.05 1.46 5.06 -1.10 -0.70 10.72)+(2×C _B -(C) -Residual	47OSB/GIN 69STU/WES 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO 43PIT/SCO C ₈ H ₁₆ ((C _B) ₂), σ = 18 Reference
Toluene $(1 \times C - (I \times C)))))))))))))))))))))$	50.00 103.64 320.66	50.43 103.53 318.36 -244.10 123.21 -49.70 12.35 159.98 208.15 -354.31 117.99	- 0.43 0.11 2.30 - 0.34 - 2.75	Reference 47OSB/GIN 69STU/WES 69STU/WES 69GOO/SMI 62SCO/GUT	$\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = $ 1,4-Dimethy (2×C-(F)) Gas phase $\Delta_t H^\circ - C_\rho^\circ = S^\circ = C_\rho^\circ = S^\circ = C_\rho^\circ = S^\circ = C_\rho^\circ = S^\circ = S$	17.32 127.57 357.69 se -25.36 183.18 253.80 Albenzene (1) ₃ (C)) + (4 Literatur 18.03 126.86	17.37 126.11 352.63 -346.15 120.57 -48.64 -24.26 183.88 243.08 -455.69 111.61 -45.02 × C _B -(H)(C _B) ₂ re Calculated 18.00 125.40	-0.05 1.46 5.06 -1.10 -0.70 10.72)+(2×C _B -(C) - Residual	47OSB/GIN 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO 43PIT/SCO 43PIT/SCO 43PIT/SCO 47OSD/GIN 69STU/WES
Toluene $(1 \times C - (I \times C))))))))))))))))))))$ $ = C_{i} = C_{i$	50.00 103.64 320.66	50.43 103.53 318.36 -244.10 123.21 -49.70 12.35 159.98 208.15 -354.31 117.99	- 0.43 0.11 2.30 - 0.34 - 2.75	Reference 47OSB/GIN 69STU/WES 69STU/WES 69GOO/SMI 62SCO/GUT	$\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = 1,4-Dimethy (2 × C-(H))$ Gas phase $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} $	17.32 127.57 357.69 se -25.36 183.18 253.80 dbenzene (1) ₃ (C)) + (4 Literatur	17.37 126.11 352.63 -346.15 120.57 -48.64 -24.26 183.88 243.08 -455.69 111.61 -45.02 × C _B -(H)(C _B) ₂ ve Calculated 18.00 125.40 352.63	-0.05 1.46 5.06 -1.10 -0.70 10.72)+(2×C _B -(C) -Residual	47OSB/GIN 69STU/WES 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO 43PIT/SCO C ₈ H ₁₆ ((C _B) ₂), σ = 18 Reference
Toluene $(1 \times C - (I \times C))))))))))))))))))))$ $ = C_{i} = C_{i$	50.00 103.64 320.66	50.43 103.53 318.36 -244.10 123.21 -49.70 12.35 159.98 208.15 -354.31 117.99	- 0.43 0.11 2.30 - 0.34 - 2.75	Reference 47OSB/GIN 69STU/WES 69STU/WES 69GOO/SMI 62SCO/GUT	$\Delta_{t}H^{\circ} = C_{r}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = C_{r}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = 1,4-Dimethy (2 × C-(H))$ Gas phase $\Delta_{t}H^{\circ} = C_{r}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = 1$	17.32 127.57 357.69 se -25.36 183.18 253.80 Albenzene (1) ₃ (C)) + (4 Literatur 18.03 126.86	17.37 126.11 352.63 - 346.15 120.57 - 48.64 - 24.26 183.88 243.08 - 455.69 111.61 - 45.02 × C _B -(H)(C _B) ₂ c Calculated 18.00 125.40 352.63 - 346.15	-0.05 1.46 5.06 -1.10 -0.70 10.72)+(2×C _B -(C) - Residual	47OSB/GIN 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO 43PIT/SCO 43PIT/SCO 43PIT/SCO 47OSD/GIN 69STU/WES
Toluene $(1 \times C - (I \times C))))))))))))))))))))$ $ = C_{i} = C_{i$	50.00 103.64 320.66	50.43 103.53 318.36 -244.10 123.21 -49.70 12.35 159.98 208.15 -354.31 117.99	- 0.43 0.11 2.30 - 0.34 - 2.75	Reference 47OSB/GIN 69STU/WES 69STU/WES 69GOO/SMI 62SCO/GUT	$\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = 1,4-Dimethy (2 × C-(H))$ Gas phase $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} $	17.32 127.57 357.69 se -25.36 183.18 253.80 Albenzene (1) ₃ (C)) + (4 Literatur 18.03 126.86	17.37 126.11 352.63 -346.15 120.57 -48.64 -24.26 183.88 243.08 -455.69 111.61 -45.02 × C _B -(H)(C _B) ₂ ve Calculated 18.00 125.40 352.63	-0.05 1.46 5.06 -1.10 -0.70 10.72)+(2×C _B -(C) - Residual	47OSB/GIN 69STU/WES 69STU/WES 45PRO/GIL 43PIT/SCO 43PIT/SCO 43PIT/SCO 43PIT/SCO 47OSD/GIN 69STU/WES

TABLE 10. Aromatic CH-01 (42) - Continued

1,4-Dimethy (2 × C-(H		× C _B −(H)(C _B) ₂)+(2×C _B -(C	C_8H_{10} C)(C _B) ₂), $\sigma = 18$		(C) + (3	$\times C_B-(H)(C_B)_2$	$(2) + (3 \times C_B - (C_B))$	C_9H_1 $C)(C_B)_2) +$
-	Literature	e – Calculated :	= Residual	Reference	(3×meta	corr), σ =	162 re – Calculated	= Residual	Reference
Liquid phas	ce ce								
$\Delta_t H^\circ = V$ $C_p^\circ = V$	-24.35 183.76	-24.26 183.88	-0.09 -0.12	45PRO/GIL 43PIT/SCO	Gas phase $\Delta_t H^\circ =$	- 15.94	-16.32	0.38	47OSB/GIN
S° =	243.51	243.08	0.43	43PIT/SCO	$C_p^{\circ} =$	150.25	149.40	0.85	69STU/WES
$\Delta_f S^\circ = \Delta_f G^\circ =$		- 455.69 111.61			$S^{\circ} = \Delta_{f}S^{\circ} =$	385.30	377.76 - 457.33	7.54	69STU/WES
$\ln K_{\rm f} =$		- 45.02			$\Delta_{\mathbf{f}}G^{\circ} =$		- 457.33 120.03		
					$\ln K_{\rm f} =$		-48.42		
1 2 3-Trime	ethylbenzene			C ₉ H ₁₂	Liquid pha				
		$\times C_{B}$ -(H)(C_{B}) ₂)+(3×C _B -(0		$\Delta_i H^\circ =$	- 63.43	-60.87	-2.56	45JOH/PRO
		meta corr), o		·)(-b)2)	$C_p^{\circ} =$	209.53	207.78	1.75	55TAY/KIL
,		ŕ			<i>s</i> ° =	273.55	278.01	-4.46	55TAY/KIL
	Literatur	e – Calculated:	= Residual	Reference	$\Delta_{\mathbf{f}}S^{\circ} =$		-557.08		
				,	$\Delta_{\mathbf{f}}G^{\circ} =$		105.22		
Gas phase					$lnK_f =$		- 42.45		
$\Delta_i H^\circ =$	- 9.46	- 12.54	3.08	47OSB/GIN					
$C_p^{\circ} =$	154.18	160.78	-6.60	69STU/WES					
S° =	384.84	381.89	2.95	69STU/WES	1,2,3,4-Tetr	amethylben	zene		C ₁₀ H ₁₄
$\Delta_f S^\circ =$		-453.19			(4 × C-(I	1)3(C))+(2	$\times C_B-(H)(C_B)_2$	$+(4\times C_{B}-(C_{B})$	
$\Delta_{\rm f}G^{\circ} =$		122.58			(3×ortho	corr)+(2	<meta corr),="" td="" σ<=""/> <td>= 162</td> <td></td>	= 162	
$\ln K_{\rm f} =$		- 49.45				T !***		D - 211	D (
		***************************************				Literatur	e – Calculated	= Kesiduai	Reference
Liquid phat $\Delta_t H^\circ =$	se - 58.53	- 54.35	-4.18	45JOH/PRO	Gas phase				
$C_p^{\circ} =$	216.44	214.78	1.66	55TAY/JOH	$\Delta_t H^{\circ} =$	-41.92	-44.34	2.42	69STU/WES
S° =	267.94	278.01	- 10.07	55TAY/JOH	$C_p^{\circ} =$	189.58	189.76	-0.18	69STU/WES
$\Delta_f S^\circ =$		-557.08			S° =	416.52	413.66	2.86	69STU/WES
$\Delta_{\rm f}G^{\circ} =$		111.74			$\Delta_f S^\circ =$		-557.74		
$lnK_f =$		- 45.08		· - · · ·	$\Delta_f G^\circ = \ln K_f =$		121.95 49.19		
1 2 4-Trime	ethylbenzene			C ₉ H ₁₂	Liquid phas	ge .			
		$\times C_B - (H)(C_B)_2$	$(2) + (3 \times C_B - (0))$		$\Delta_{i}H^{\circ} =$	- 90.21	-87.70	-2.51	75GOO
		«meta corr), σ			$C_p^{\circ} =$	235.98	242.18	-6.20	31HUF/PAR
					S° =	290.79	312.94	-22.15	31HUR/PAR
	Literatur	e - Calculated	= Residual	Reference	$\Delta_f S^\circ =$		-658.46		
					$\Delta_f G^\circ = \ln K_f =$		108.62 43.82		
Gas phase					111Kf -		-43.82		
$\Delta_t H^\circ =$	- 13.85	- 13.80	-0.05	47OSB/GIN					
$C_p^{\circ} =$	154.01	154.38	-0.37	69STU/WES					
S° =	395.76	390.16	5.60	69STU/WES	1,2,3,5-Tetr				C10H14
$\Delta_{\mathbf{f}}S^{\circ} =$		- 444.93					$\times C_B-(H)(C_B)_2$		$(C_B)_2) +$
$\Delta_{\rm f}G^{\circ} =$		118.86			(2×ortho	corr)+(2>	meta corr), o	= 162	
		- 47.95				Literatur	e – Calculated	= Residual	Reference
$\ln K_{\rm f} =$									
$lnK_f =$	se		-4.19	45JOH/PRO	Gas phase				
	nse 61.80	-57.61			$\Delta_{\ell}H^{\circ} =$	-44.81	-45.60	0.79	COCTLIANTE
$lnK_f =$ Liquid pha		- 57.61 211.28	3.69	57PUT/KIL	$\Delta \mu_I -$	77.01		0.77	69STU/WES
$lnK_f =$ Liquid pha $\Delta_f H^\circ =$	-61.80			57PUT/KIL 57PUT/KIL		185.73	183.36	2.37	69STU/WES
In $K_f =$ Liquid pha $\Delta_f H^\circ =$ $C_f^\circ =$ $S^\circ =$ $\Delta_f S^\circ =$	- 61.80 214.97	211.28	3.69		$C_p^{\circ} = S^{\circ} =$				
Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	- 61.80 214.97	211.28 278.01 - 557.08 108.48	3.69		$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} =$	185.73	183.36	2.37	69STU/WES
In $K_f =$ Liquid pha $\Delta_f H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_f S^\circ =$	- 61.80 214.97	211.28 278.01 - 557.08	3.69		$C_p^{\circ} = S^{\circ} =$	185.73	183.36 416.16	2.37	69STU/WES

,	0011)	meta corr), σ			(×meta corr), o		
·	Literature	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid phas	e				Liquid pha	se			
$\Delta_t H^\circ =$	- 96.36	90.96	-5.40	75GOO	$\Delta_{\rm f}H^{\rm o} =$	- 122.97	- 121.05	-1.92	33FER/THO
$C_p^{\circ} =$	240.16	238.68	1.48	31HUF/PAR	$C_p^{\circ} =$		269.58		
s° =	310.03	312.94	- 2.91	31HUF/PAR	s° =		347.87		
$\Delta_f S^\circ =$		658.46			$\Delta_{\mathbf{f}}S^{\circ} =$		<i>−</i> 759.84		
$\Delta_{\mathbf{f}}G^{\circ} =$		105.36			$\Delta_f G^\circ =$		105.50		
$lnK_f =$		- 42.50			$lnK_f =$		- 42.56		
					Solid phase	e			
1.2.4.5-Tetra	amethylbenz	zene		$C_{10}H_{14}$	$\Delta_t H^{\circ} =$	-133.64	- 129.67	-3.97	64BON/COL
		$\times C_B - (H)(C_B)_2$	$(4 \times C_{B} - (0))$		$C_p^{\circ} =$	270.29	241.08	29.21	44EIB
		meta corr), o			S° =	294.14	278.70	15.44	31HUF/PAR
•	, ,	•			$\Delta_{\mathbf{f}}S^{\circ} =$		-829.01		
	Literatur	e – Calculated	= Residual	Reference	$\Delta_{\mathbf{f}}G^{\circ} =$		117.50		
		· ————————————————————————————————————			$lnK_t =$		-47.40		
Gas phase	45.27	- 45.60	0.33	69STU/WES					
$\Delta_{\mathfrak{l}}H^{\circ} =$	- 45.27 186.52	- 45.60 183.36	3.16	69STU/WES	Hexamethy	lhenzene			C12H1
$C_{\rho}^{\circ} = S^{\circ} =$			8.13	69STU/WES			× C =(C)(C)) i (6 v owho	
$\Delta_t S^\circ =$	418.53	410.40 -561.00	0.13	03310/WE3		$corr$), $\sigma =$	$6 \times C_B - (C)(C_B)$)+(u×onno ((OII) +
$\Delta_f S^\circ = \Delta_f G^\circ = 0$		-301.00 121.66			(3×meiu	(011), 0 -	0/40		
$\ln K_{\rm c} =$		- 49.08				T itamatu	re – Calculated	_ Dooldwal	Reference
mx _t =		- 49.08				Literatu		- Kesiduai	Keterence
Liquid phas	se				Gas phase				
$\Delta_i H^\circ =$	- 98.99	- 90.96	-8.03	75GOO	$\Delta_{\rm f}H^{\circ} =$	- 86.82	- 107.31	20.49	67FRA/AST
$C_p^{\circ} =$		238.68			$C_p^{\circ} =$	248.61	254.83	-6.22	69STU/WES
S° =		312.94			s° =	452.37	459.79	- 7.42	69STU/WES
$\Delta_f S^\circ =$		- 658.46			$\Delta_{\rm f} S^{\circ} =$		<i>−</i> 784.23		
$\Delta_t G^{\circ} =$		105.36			$\Delta_{t}G^{\circ} =$		126.51		
$lnK_f =$		- 42.50			$lnK_{\ell} =$		-51.03		
Solid phase					Liquid phas	se			
•	-119.87	- 104.30	~ 15.57	75GOO	$\Delta_{\rm f}H^{\circ} =$	- 139.14	- 151.14	12.00	32SPA/THO
$C_p^o =$	220.08	217.02	3.06	44EIB	$C_p^{\circ} =$		300.48		0-0-1-4-1-10
s° =	245.60	250.26	- 4.66	31HUF/PAR	S° =		382.80		
$\Delta_f S^\circ =$		-721.14			$\Delta_{f}S^{\circ} =$		-861.22		
$\Delta_{\mathbf{f}}G^{\circ} =$		110.71			$\Delta_t G^{\circ} =$		105.63		
$lnK_f =$		- 44.66			$lnK_f =$		-42.61		
					Solid phase				
Pentamethy	lhenzene			$C_{11}H_{16}$	$\Delta_{\rm f}H^{\circ} =$	- 161.54	- 157.04	-4.50	64BON/COL
		$\times C_B$ -(H)(C _B) ₂	1)+(5×C(C		$C_p^{\circ} =$	245.64	265.14	- 19.50	65FRA/AST
		meta corr), o		,,, - 2 ,2, ,	S° =	306.31	307.14	-0.83	65FRA/AST
((()		100		$\Delta_{f}S^{\circ} =$	500.51	-936.88	0.05	OSI KAYASI
	Literatur	e – Calculated	= Residual	Reference	$\Delta_{\rm f}G^{\circ} =$		122.29		
			10514441		$\ln K_{\rm f} =$		-49.33		
Gas phase		.							
$\Delta_i H^\circ =$	- 74.48	- 76.77	2.29	69STU/WES					
$C_p^{\circ} =$	216.48	219.45	-2.97	69STU/WES					
	443.88	445.42	- 1.54	69STU/WES					
S° =	443.00		1.57	0751071125					
$\Delta_f S^\circ =$	443.00	-662.28	1.54	0,510, W25					
-	443.00		1.54	0,510,4125					

TABLE 10. Aromatic CH-01 (42) - Continued

	ne [) ₃ (C))+(1> H)(C _B) ₂), σ	$C-(H)_2(C)(C)$ = 6	(B)) + $(1 \times C_B -$	$(C)(C_B)_2) +$		$I_{3}(C) + (2$	ed) \times C(H) ₂ (C) ₂) - $(5 \times C_B$ (H)(C _B)		$(C)(C_B)) +$
	Literature	e – Calculated =	= Residual	Reference		Literatur	e – Calculated =	= Residual	Reference
Gas phase					Liquid phas				
$\Delta_i H^\circ =$	29.92	29.09	0.83	47OSB/GIN	$\Delta_f H^{\circ} =$	-63.85	-63.92	0.07	46PRO/JOH
$C_p^{\circ} =$	128.41	129.14	-0.73	69STU/WES	$C_p^{\circ} =$	243.34	243.72	-0.38	65MES/TOD
S° =	360.45	360.95	-0.50	69STU/WES	<i>S</i> ° =	321.21	320.31	0.90	65MES/TOD
$\Delta_f S^\circ =$		-337.82			$\Delta_f S^\circ =$		-651.09		
$\Delta_{\rm f}G^{\circ} =$		129.81			$\Delta_{\mathbf{f}}G^{\circ} =$		130.20		
$lnK_f =$		- 52.37			$lnK_f =$		-52.52		
Liquid phas	se								
$\Delta_t H^\circ =$	-12.34	- 12.46	0.12	45PRO/GIL	Pentylbenze	ene			$C_{11}H_{16}$
$C_p^{\circ} =$	185.81	182.88	2.93	44GUT/SPI	•		\times C-(H) ₂ (C) ₂) -	+ (1 × C-(H)-	
S° =	255.01	255.55	-0.54	44GUT/SPI			$(5 \times C_{R} - (H)(C_{R})$		· · · · · · · · · · · · · · · · · · ·
$\Delta_f S^\circ =$		-443.22		-			. , , , , , , ,		
$\Delta_f G^\circ = \ln K_f =$		119.69 48.28				Literatur	e – Calculated :	= Residual	Reference
mel _		70.20			G- :				
					Gas phase	24.42	20.00	1.62	COOTTIATEO
n 11				0.11	$\Delta_{\mathbf{f}}H^{\circ} =$	-34.43	-32.80	-1.63	69STU/WES
Propylbenz			. (1(2.(11)	C ₉ H ₁₂	$C_p^{\circ} = .$	197.99	197.81	0.18	69STU/WES
		\times C-(H) ₂ (C) ₂)		(C)(C _B))+	.ς° = Δ _t ς° =	478.94	478.43 629.28	0.51	69STU/WES
(1 × CB-($(C)(C_B)_2)+($	$(5 \times C_B - (H)(C_B))$	$_{3})_{2}), \sigma = 0$		$\Delta_{f}S = \Delta_{f}G^{\circ} =$		154.82		
	I itarat	e - Calculated	- Residual	Reference	$\Delta_f G^* = \ln K_f =$		- 62.45		
	Literatur	- Calculated	- residuai	Reference	ink _f =		- 02.43		
Gas phase					Liquid phas	se			
$\Delta_i H^{\circ} =$	7.91	8.46	-0.55	47OSB/GIN	$\Delta_{\mathbf{f}}H^{\circ} =$		-89.65		
$C_p^{\circ} =$	152.34	152.03	0.31	69STU/WES	$C_p^{\circ} =$		274.14		
S° =	400.66	400.11	0.55	69STU/WES	<i>s</i> ° =		352.69		
$\Delta_f S^\circ =$		- 434.97			$\Delta_f S^\circ =$		-755.02		
$\Delta_f G^\circ =$		138.15			$\Delta_{\rm f}G^{\circ} =$		135.46		
lnK₁ −		- 55.73			$lnK_r =$		- 54.64		
T::d -L-									
Liquid pha $\Delta_r H^\circ =$	-38.33	- 38.19	-0.14	45PRO/GIL	Hexylbenze			1 - 1	C ₁₂ H ₁₆
$C_p^{\circ} =$	214.72	213.30	1.42	65MES/TOD	(1×C-(I	1) ₃ (C)) + (4	\times C-(H) ₂ (C) ₂) -	$+(1\times C-(H)_2)$	$(C)(C_B)) +$
S° =	287.78	287.93	-0.15	65MES/TOD	$(1 \times C_B - ($	$C)(C_B)_2)+($	$(5 \times C_B - (H)(C_B))$	$)_2), \sigma = 6$	
$\Delta_{\rm f} S^{\circ} =$		-547.16				T :++	o Coloulata	- Dooldwal	Doforce
$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = $		124.94 50.40				Literatur	e – Calculated =	- residual	Reference
					Gas phase				
					$\Delta_{i}II^{\circ}$ —	-55.02	−53.43	- 1.59	69STU/WES
Butylbenze	ne			C ₁₀ H ₁₄	$C_p^{\circ} =$	220.87	220.70	0.17	69STU/WES
(1×C-(1	$H)_3(C)) + (2$	\times C-(H) ₂ (C) ₂)	$+(1\times C-(H)_2$		<i>S</i> ° =	517.90	517.59	0.31	69STU/WES
		$(5 \times C_{B} - (H)(C_{E})$		•	$\Delta_f S^\circ =$		-726.43		
					$\Delta_f G^\circ =$		163.15		
	Literatu	re – Calculated	= Residual	Reference	$lnK_f =$		- 65.82		
					Tionid -t-				
Gos ak		10 17	_ 0.00	ACDROJICII	Liquid phas	50	_115 20		
	-13.05	12.17 174.92	- 0.88 0.18	46PRO/JOH 69STU/WES	$\Delta_{\mathbf{f}}H^{\circ} = C_{p}^{\circ} =$		-115.38 304.56		
$\Delta_{\rm f}H^{\circ} =$	175 10	1/4.74							
$\Delta_{i}H^{\circ} = C_{p}^{\circ} =$	175.10 430 40	430.27	በ 22	60CTH/W/EC					
$\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} =$	175.10 439.49	439.27 - 532.12	0.22	69STU/WES	S° =		385.07 -858.95		
$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} =$		-532.12	0.22	69STU/WES	$\Delta_t S^\circ =$		-858.95		
$\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} =$			0.22	69STU/WES					

	(C) + (5	× C-(H) ₂ (C) ₂) - (5 × C _B -(H)(C _B		$C_{13}H_{20}$ $(C)(C_B)) +$		$H_{3}(C)) + (7$	ued) '× C-(H) ₂ (C) ₂) (5 × C _B -(H)(C ₁		$C_{15}H_{24}$ (C)(C _B))+
	Literatur	e – Calculated :	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$	- 75.65 243.72 556.85	-74.06 243.59 556.75 -823.58 171.49 -69.18	-1.59 0.13 0.10	69STU/WES 69STU/WES 69STU/WES	Liquid pha $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se	-192.57 395.82 482.21 -1170.74 156.49 -63.13		
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S$	se	- 141.11 334.98 417.45 - 962.88 145.97				$(C)(C_B)_2$	5 × C-(H) ₂ (C) ₂) (5 × C _B -(H)(C ₁ re – Calculated	$(\alpha_3)_2$), $\sigma = 6$	$C_{16}H_{26}$ $(C)(C_B)) +$ Reference
	$(C)(C_B)_2$	-58.88 × C-(H) ₂ (C) ₂) (5 × C _B -(H)(C _B) re - Calculated	$(a)_2$), $\sigma = 6$	$C_{14}H_{22}$ $(C)(C_B)) +$ Reference	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 137.49 312.34 673.71	-135.95 312.26 674.23 -1115.03 196.50 -79.27	-1.54 0.08 -0.52	69STU/WES 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t =$	- 96.23 266.60 595.80	- 94.69 266.48 595.91 - 920.73 179.83 - 72.54	-1.54 0.12 -0.11	69STU/WES 69STU/WES 69STU/WES	Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se	-218.30 426.24 514.59 -1274.67 161.74 -65.25		
Liquid pha $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	ise	166.84 365.40 449.83 1066.81 151.23 61.01				$(C)(C_B)_2 + (S_B)_2$	\times C-(H) ₂ (C) ₂) (5 \times C _B -(H)(C _E) re – Calculated	$(3)_2$), $\sigma = 6$	$C_{17}H_{28}$ $(C)(C_B)) +$ Reference
Nonyibenze (1×C-(1	$H)_3(C)) + (7$ $(C)(C_B)_2) +$	$F \times C$ - $(H)_2(C)_2$) $(5 \times C_B$ - $(H)(C_B$) F = -C	$(3)_2$), $\sigma = 6$	$C_{15}H_{24}$ $(C)(C_B)) +$ Reference	Gas phase $ \Delta_{\mathbf{f}}H^{\circ} = \\ C_{\rho}^{\circ} = \\ S^{\circ} = \\ \Delta_{\mathbf{f}}S^{\circ} = \\ \Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = \\ $	- 158.07 335.22 712.62	-156.58 335.15 713.39 -1212.18 204.83 -82.63	- 1.49 0.07 - 0.77	69STU/WES 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-116.86 289.45 634.75	-115.32 289.37 635.07 -1017.88 188.16 -75.90	-1.54 0.08 -0.32	69STU/WES 69STU/WES 69STU/WES	Liquid pha $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se	-244.03 456.66 546.97 -1378.60 167.00 -67.37		

TABLE 10. Aromatic CH-01 (42) - Continued

	() ₃ (C))+(10)	\times C-(H) ₂ (C) ₂) \times C _B -(H)(C _B)		$C_{18}H_{30}$ $C(C)(C_B)) +$	(2×C-(I	(C) + (1)	e (Continued) × C-(H) ₂ (C)(C (1×meta corr)		C_9H_{12} (C)(C _B) ₂)+
	Literature	– Calculated =	Residual	Reference	·	Literatur	c – Calculated	- Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t =$	- 178.70 358.07 751.57	-177.21 358.04 752.55 -1309.33 213.17 -85.99	-1.49 0.03 -0.98	69STU/WES 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = In K_f =$	se - 48.70	- 49.07 206.78 290.48 - 544.61 113.30 - 45.71	0.37	45JOH/PRO
Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $		- 269.76 487.08 579.35 - 1482.54 172.26 - 69.49			(2×C-(I	(H)(C _B) ₂), σ	× C-(H) ₂ (C)(C		C_3H_{12} $(C)(C_B)_2) +$ Reference
(2×C-(F	$(H)(C_B)_2)+(1$	e < C-(H) ₂ (C)(C ₁ 1× <i>ortho</i> corr), e – Calculated =	$\sigma = 9$	C_9H_{12} $(C)(C_B)_2) +$ Reference	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = $	- 3.26 151.54 398.90	-3.34 151.01 395.22 -439.87 127.81 -51.56	0.08 0.53 3.68	69STU/WES 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	1.21 157.90 399.24	-2.08 157.41 398.48 -436.60 128.09 -51.67	3.29 0.49 0.76	69STU/WES 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	se 49.79	-49.07 206.78 290.48 -544.61 113.30 -45.71	-0.72	45JOH/PRO
Liquid phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se 46.40	- 45.81 210.28 290.48 - 544.61 116.56 - 47.02	- 0.59	45JOH/PRO	(2×C-(I	$C)(C_B)_2) + ($	ene × C-(H) ₂ (C) ₂) 4 × C _B -(H)(C _B e – Calculated	$(1 \times ortho$	
(2×C-(I	$(H)(C_B)_2)+($	e ×C-(H) ₂ (C)(C 1× <i>meta</i> corr), e - Calculated =	$\sigma = 9$	C_9H_{12} $(C)(C_B)_2) +$ Reference	Gas phase $ \Delta_t H^\circ = C_p^\circ = $ Liquid phas $ \Delta_t H^\circ = $	se 72.47	-22.71 180.30	-0.93	73GOO
Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ - \Delta_t G^\circ = \ln K_t = $	- 1.92 152.21 404.17	- 3.97 151.72 400.98 - 434.10 125.46 - 50.61	2.05 0.49 3.19	69STU/WES 69STU/WES 69STU/WES	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = -\infty$		240.70 322.86 648.54 121.82 49.14		

(2×C-(H	propylbenzene $(C)(C_B)_2 + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2) + (1 \times C_B - (H)_2(C)_2)$			$(1 \times C - (H)(C)_2(C_B)) +$ ertiary)) + $(2 \times C_B - (C)(C_B)_2) +$	C ₁₀ H ₁₄
	Literature - Calculated = Residual	Reference	Litera	Reference	
Gas phase					
$\Delta_t H^\circ =$	-24.60		Gas phase	44.00	
C _p =	174.61		$\Delta_t H^\circ = C_p^\circ =$	-33.93 174.29	
Liquid phas $\Delta_t H^\circ =$	e -76.23 -74.80 -1.43	73GOO	Liquid phase		
		/3G00	$\Delta_t H^\circ = -78.62$	-82.05 3.43	73GOO
$C_p^{\circ} =$	237.20		$C_p^{\alpha} = -76.02$	237.86	/3000
$S^{\circ} = \Delta_{f}S^{\circ} =$	322.86 648.54		$S^{\circ} =$	312.48	
$\Delta_f S^\circ = \Delta_f G^\circ =$	118.56		$\Delta_t S^\circ =$	-658.92	
			$\Delta_{\mathbf{f}}G^{\circ} =$	114.41	
$lnK_f =$	-47.83 		$lnK_f =$	-46.15	
(2 × C-(I	propylbenzene $1_{3}(C)$) + $(1 \times C - (H)_2(C)_2)$ + $(1 \times C - (H)_2(C)_2)$ $(1 \times C - (H)_2(C)_2)$ + $(1 \times C - (H)_2(C)_2)$	$C_{10}H_{14}$ $C)(C_B)) +$	1-Methyl-4-isopropy (3×C-(H) ₃ (C))+	Thenzene $(1 \times C - (H)(C)_2(C_B)) +$	C ₁₀ H ₁₄
, - ,	, -,-, , , , , , , , , , , , , , , , ,			ertiary)) + $(2 \times C_B - (C)(C_B)_2)$ +	
	Literature – Calculated = Residual	Reference	$(4 \times C_B - (H)(C_B)_2)$ Litera) ture – Calculated = Residual	Reference
Gas phase	22.07		Can abasa		
$\Delta_i H^\circ =$	-23.97 173.00		Gas phase $\Delta_t II^\circ =$	-33.30	
C _p =	173.90		$C_p^{\circ} =$	-33.30 173.58	
Liquid pha	se.		***************************************		· · · · · · · · · · · · · · · · · · ·
$\Delta_t H^\circ =$	-75.06 -74.80 -0.26	73GOO	Liquid phase		
$C_p^{\circ} =$	237.20	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	$\Delta_t H^\circ = -78.03$	-82.05 4.02	73GOO
S° =	322.86		$C_p^{\circ} = 236.40$	-	31HUF/PAR
$\Delta_f S^\circ =$	-648.54		$S^{\circ} = 306.69$		31HUF/PAR
$\Delta_{\mathbf{f}}G^{\circ} =$	118.56		Δ _f S°	-658.92	311101/17IIX
$lnK_f =$	-47.83		$\Delta_{\rm f}G^{\circ} =$	114.41	
			$\ln K_{\rm f} =$	-46.15	
(3×C-(I (2×-CH	isopropylbenzene $H_{3}(C)$ + $(1 \times C - (H)(C)_2(C_B))$ + $(1 \times C - (H)(C)_2(C_B)$ + $(1 \times C)_2(C)$ + $(1 \times C)_3(C)$ + $(1 \times C)_3(C)$ + $(1 \times C)_3(C)$ + $(1 \times C)_3(C)$ + $(1 \times C)_3(C)$ + $(1 \times C)_3(C)$	C ₁₀ H ₁₄	3-Ethyl-1,2-dimethyl (3×C-(H) ₃ (C)) + (3×C _B -(H)(C _B) ₂)	benzene $(1 \times C - (H)_2(C)(C_B)) + (3 \times C_{B^-}) + (2 \times ortho \text{ corr}) + (1 \times meta \text{ corr})$	$C_{10}H_{14}$ (C)(C _B) ₂) +
, -,	Literature - Calculated = Residual	Reference		ture – Calculated = Residual	Reference
Gas phase	22.04		Gas phase	22.60	
$\Delta_{\rm f}H^{\circ} =$	-32.04 170.00		$\Delta_t H^\circ =$	-33.88	
~~	179.98		$C_p^{\circ} =$	186.39	
$C_p^{\circ} =$					
	SC		Liquid phase		
Liquid pha		73GOO	Liquid phase $\Delta_t H^\circ = -80.50$	-79.16 -1.34	75GOO
Liquid pha $\Delta_l H^\circ =$	se -73.30 -78.79 5.49 241.36	73GOO	Liquid phase $\Delta_t H^\circ = -80.50$ $C_p^\circ =$	-79.16 -1.34 237.68	75GOO
Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ =$	−73.30 −78.79 5.49	73GOO	$\Delta_{\rm f}H^{\circ} = -80.50$		75GOO
Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ =$	-73.30 -78.79 5.49 241.36	73GOO	$\Delta_{\rm f}H^{\circ} = -80.50$ $C_{\rm p}^{\circ} =$	237.68	75GOO
Liquid pha $\Delta_t H^\circ = C_p^\circ =$	-73.30 -78.79 5.49 241.36 312.48	73GOO	$\Delta_t H^\circ = -80.50$ $C_p^\circ = S^\circ =$	237.68 325.41	75GOO

(3×C-(F	dimethylbenzene $H_{3}(C)$) + $(1 \times C-(H)_{2}(C)(C_{B}))$ + $(3 \times C_{B}-(H)(C_{B})_{2})$ + $(1 \times ortho\ corr)$ + $(1 \times meta\ corr)$		5-Ethyl-1,3-dimethylb $(3 \times C - (H)_3(C)) + ($ $(3 \times C_B - (H)(C_B)_2) - $	$1 \times C - (H)_2(C)(C_B)) + (3 \times C_B -$	$(C)(C_B)_2) +$
	Literature - Calculated = Residual	Reference	Literati	ure – Calculated = Residual	Reference
Gas phase			Gas phase		
$\Delta_{f}H^{\circ} = $			$\Delta_{\rm f}H^{\circ} =$	-37.66	
$C_p^{\circ} =$	179.99		$C_p^{\circ} =$	175.01	
Liquid phas	se		Liquid phase		
$\Delta_t H^\circ =$	-86.02 -82.42 -3.60	75GOO "	$\Delta_{\rm f}H^{\circ} = -87.78$	-85.68 -2.10	75GOO
$C_p^{\circ} =$	234.18		$C_p^{\circ} =$	230.68	
S° =	325.41		S° =	325.41	
$\Delta_f S^\circ =$	-645.99		$\Delta_{\mathbf{f}}S^{\circ} =$	- 645.99	
$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = $	110.18 44.45		$\Delta_f G^\circ = \ln K_f =$	106.92 - 43.13	
(3×C-(I	-dimethylbenzene $H_{13}(C)$) + $(1 \times C - (H)_2(C)(C_B))$ + $(3 \times C_B - (H)(C_B)_2)$ + $(2 \times ontho \ corr)$ + $(1 \times meta \ co$ Literature – Calculated = Residual		$(3\times C_B-(H)(C_B)_2)$	$1 \times C - (H)_2(C)(C_B)) + (3 \times C_{B^-} + (1 \times ortho \text{ corr}) + (1 \times meta \text{ corr})$ $- Calculated = Residual$	
Gas phase	22.00		Gas phase	25.14	
$\Delta_t H^\circ = C_p^\circ =$	- 33.88 186.39		$\Delta_{\ell}H^{\circ} = C_{p}^{\circ} =$	-35.14 179.99	
Liquid pha	se		Liquid phase		
$\Delta_t H^\circ =$	-80.12 -79.16 -0.96	75GOO	$\Delta_t H^\circ = -84.81$	-82.42 -2.39	75GOO
$C_p^{\circ} =$	237.68		$C_p^{\circ} =$	234.18	
S° =	325.41		S° =	325.41	
$\Delta_f S^\circ =$	-645.99		$\Delta_{f}S^{\circ} =$	645.99	
$\Delta_f G^\circ =$	113.44		$\Delta_{\mathbf{f}}G^{\circ} =$	110.18	
$lnK_t =$	-45.76		$lnK_f =$	-44.45	
(3×C-(I	-dimethylbenzene H) ₃ (C)) + (1 × C-(H) ₂ (C)(C _B)) + (3 × C _B -(2×C-(H) ₂ (C)(C _B))+(2×C _B -($C_{10}H_{14}$ (C)(C _B) ₂) +
(3×C _B -($(H)(C_B)_2$ + $(1 \times ortho \ corr)$ + $(1 \times meta \ corr)$		$(4 \times C_B - (H)(C_B)_2) +$		
	Literature - Calculated = Residual	Reference	Literatu	ere – Calculated = Residual	Reference
Gas phase			Gas phase		
$\Delta_f H^\circ =$	-35.14		$\Delta_t H^{\circ} =$	-23.42	
$C_p^{\circ} =$	179.99		$C_p^{\circ} =$	183.02	·
Liquid pha			Liquid phase		
	-84.10 -82.42 -1.68	75GOO	$\Delta_t H^{\circ} = -68.49$	-70.62 2.13	75GOO
$\Delta_t H^\circ =$			$C_p^{\circ} =$	233.18	
$\Delta_{\mathbf{f}}H^{\circ} = C_{p}^{\circ} =$	234.18				
$\Delta_t H^\circ = C_p^\circ = S^\circ =$	325.41		S° =	337.88	
$\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} =$	325.41 645.99		$S^{\circ} = \Delta_{f}S^{\circ} =$	337.88 - 633.52	
$\Delta_t H^\circ = C_p^\circ = S^\circ =$	325.41		S° =	337.88	

TABLE 11. Aromatic CH-02 (80)

1,3-Diethylbenzene	C10H14
$(2 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)(C_B)) + (2 \times C_B - (C)(C_B)_2) +$	
$(4 \times C_B - (H)(C_B)_2) + (1 \times meta \text{ corr})$	

	Literatu	re – Calculated =	Reference		
Gas phase					
$\Delta_t H^{\circ} =$		- 25.31			
$C_p^{\circ} =$		177.33			.,
Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ $	-73.51	-73.88 229.68 337.88	0.37	73GOO	
$\Delta_f S^\circ =$		-633.52			
$\Delta_{\mathbf{f}}G^{\circ} =$		115.00			
$lnK_f =$		- 46.39			

1,4-Diethylbenzene

 $C_{10}H_{14}$ $(2 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)(C_B)) + (2 \times C_B - (C)(C_B)_2) + (4 \times C_B - (H)(C_B)_2), \sigma = 18$

	Literatur	e – Calculated	= Residual	Reference		
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	176.15 434.01	- 24.68 176.62 437.81 - 533.59 134.41 - 54.22	- 0.47 - 3.80	69STU/WES 69STU/WES		
Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	- 72.84	-73.88 229.68 337.88 -633.52 115.00 -46.39	1.04	73GOO		

1,2,3-Triethylbenzene	C12H18
$(3 \times C - (H)_3(C)) + (3 \times C - (H)_2(C)(C_B)) + (3 \times C_B - (C)(C_B)_2) +$	
$(3 \times C_B - (H)(C_B)_2) + (2 \times ortho \ corr) + (1 \times meta \ corr), \sigma = 54$	1

	Literatur	Reference		
Gas phase				
$\Delta_t H^\circ =$	-67.99	-76.56	8.57	69STU/WES
$C_p^o =$	228.11	237.61	-9.50	69STU/WES
S° =	507.23	509.66	-2.43	69STU/WES
$\Delta_f S^\circ =$		- 734.36		
$\Delta_{\mathbf{f}}G^{\circ} =$		142.39		
$lnK_f =$		-57.44		
Liquid pha	nca			
$\Delta_i H^\circ =$	130	- 128.78		
$C_p^{\circ} =$		283.48		
S° =		420.21		
$\Delta_{i}S^{\circ} =$		- 823.81		
$\Delta_{\rm f}G^{\circ} =$		116.84		
$lnK_f =$		-47.13		

1,2,4-Triethylbenzene $C_{12}H_{18}$ $(3 \times C - (H)_3(C)) + (3 \times C - (H)_2(C)(C_B)) + (3 \times C_B - (C)(C_B)_2) +$ $(3 \times C_B - (H)(C_B)_2) + (1 \times ortho corr) + (1 \times meta corr), \sigma = 27$

	Literatui	re – Calculated	= Residual	Reference		
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-71.09 227.94 518.15	-77.82 231.21 517.93 -726.09 138.66 -55.94	6.73 - 3.27 0.22	69STU/WES 69STU/WES 69STU/WES		
Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = 1$	se	- 132.04 279.98 420.21 - 823.81 113.58 - 45.82				

1,3,5-Triethylbenzene $C_{12}H_{18}$ $(3 \times C - (H)_3(C)) + (3 \times C - (H)_2(C)(C_B)) + (3 \times C_B - (C)(C_B)_2) +$ $(3 \times C_B - (H)(C_B)_2) + (3 \times meta \text{ corr}), \sigma = 162$

	Literatur	Literature – Calculated = Residual					
Gas phase							
$\Delta_f H^\circ =$	-74.73	-80,34	5.61	69STU/WES			
$C_p^{\circ} =$	224.18	226.23	-2.05	69STU/WES			
S° =	507.69	505.53	2.16	69STU/WES			
$\Delta_{\mathbf{f}}S^{\circ} =$		- 738.49					
$\Delta_f G^\circ =$		139.84					
$lnK_f =$		-56.41					

TABLE 11. Aromatic CH-02 (80) - Continued

$(3 \times C - (H)_3)$	benzene (Continued) $s(C) + (3 \times C - (H)_2(C)(C_B)) + (3 \times C_B)(C_B)_2 + (3 \times meta \text{ corr}), \sigma = 162$			$(1)_3(C)) + (6)$	×C-(H) ₂ (C)(C meta corr), σ		$C_{18}H_3$ (C)(C _B) ₂) +
	Literature - Calculated = Residu	al Reference		Literatur	e – Calculated	= Residual	Reference
Liquid phase			Solid phase				
$\Delta_t H^\circ =$	- 135.30		$\Delta_t H^\circ =$		-289.64		
$C_p^{\circ} =$	276.48		$C_p^{\circ} =$		561.42		
$S^{\circ} =$	420.21		S° =		468.54		
$\Delta_f S^\circ =$	-823.81		$\Delta_{\rm f}S^{\circ} =$		- 1593.34		
$\Delta_{\rm f}G^{\circ} =$	110.32		$\Delta_t G^{\circ} =$		185.42		
$\ln K_{\rm f} =$	- 44.50		$\ln K_{\rm f} =$		-74.80		
D 4 4 1		O W	T				
Pentaethylber (5×C-(H)	nzene ₃ (C)) + (5 × C-(H) ₂ (C)(C _B)) + (5 ×	$C_{16}H_{26}$ C_{B} - $(C)(C_{B})_{2}) +$		$(1)_3(C) + (1)_3(C)$	\times C-(H)(C) ₂ (C		C ₂ H ₁
$(1 \times C_B - (H$	$(C_B)_2$ + $(4 \times ortho \ corr)$ + $(4 \times max)$	eta corr), $\sigma = 486$		corr (terti H)(C _B) ₂), or	$ary)) + (1 \times C_{B} - 18)$	$(C)(C_B)_2) +$	
	Literature – Calculated = Residu	al Reference	(* -2 (, , , ,	e – Calculated =	= Residual	Reference
						- Itosiaaai	
Gas phase	477 10 103 47 0.0	0 (007) (4)					
	· 175.18 — 183.47 8.2		Gas phase	4.00	0.07	4.00	4700D/GDI
$C_p^{\circ} =$	339.70 347.50 -7.8	•	$\Delta_{\mathbf{f}}H^{\circ} =$	4.02	-0.87	4.89	47OSB/GIN
S° =	647.89 658.37 -10.4	8 69STU/WES	$C_p^{\circ} =$	151.71	151.71	0.00	69STU/WES
$\Delta_f S^\circ =$	- 1130.89		S° =	388.57	388.55	0.02	69STU/WES
$\Delta_f G^\circ =$	153.70		$\Delta_{\mathbf{f}}S^{\circ} =$		- 446.54		
$lnK_f =$	-62.00		$\Delta_f G^\circ = InK_f =$		132.27 - 53.35		
Liquid phase							
$\Delta_{\rm f}H^{\circ} =$	-245.10		Liquid phas	e			
$C_p^{\circ} =$	384.08		$\Delta_t H^\circ =$	-41.13	- 45.44	4.31	45JOH/PRO
S° =	584.87		$C_p^{\circ} =$	215.40	213.96	1.44	73KIS/SUG
$\Delta_f S^\circ =$	- 1204.39		<i>S</i> ° =	277.57	277.55	0.02	73KIS/SUG
$\Delta_{\mathbf{f}}G^{\circ} =$	113.99		$\Delta_f S^\circ =$		-557.54		
$lnK_f =$	- 45.98		$\Delta_f G^{\circ} =$		120.79		
			$lnK_f =$		-48.73		
	$_{3}(C)) + (6 \times C - (H)_{2}(C)(C_{B})) + (6 \times C - (H)_{2}(C)(C_{$	$C_{18}H_{30}$ $C_{C_{B}}(C_{C_{B}}(C_{C_{B}}))$			ne; sec-Butylbei		C10H14
(6×ortho	corr) + $(5 \times meta \text{ corr})$, $\sigma = 8748$ Literature – Calculated = Residu	al Reference		corr (terti	\times C-(H) ₂ (C) ₂) + ary)) + (1 \times C _B -		C) ₂ (C _B)) +
				Literatur	e – Calculated =	= Residual	Reference
Gas phase	224.26 225.25 11.0	0 (0071143770					
A 770	-224.26 -235.35 11.0		C 1				
-			Gas phase	177.01	40.04	4.00	ACDD OUTCOM
$C_p^{\circ} =$	396.48 408.49 -12.0	O COOPER TREESON	$\Delta_{\rm f}H^{\circ} =$	- 17.36	- 19.24 174.60	1.88	46PRO/JOH
$C_p^{\circ} = S^{\circ} =$	697.14 715.33 -18.1	9 69STU/WES	~~		174.60		
$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} =$	697.14 715.33 -18.1 -1346.55	9 69STU/WES	$C_p^{\circ} =$				
$C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{f}G^{\circ} =$	697.14 715.33 -18.1 -1346.55 166.12	9 69STU/WES	$C_p^{\circ} =$	<u> </u>			
$C_{\rho}^{\circ} = S^{\circ} = \Delta_{i}S^{\circ} = 0$	697.14 715.33 -18.1 -1346.55	9 69STU/WES	Liquid phas	e		· · · · · · · · · · · · · · · · · · ·	
$C_{\rho}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} =$	697.14 715.33 -18.1 -1346.55 166.12 -67.01	9 69STU/WES	Liquid phas $\Delta_t H^\circ =$	e -66.40	-68.99	2.59	46PRO/JOH
$C_{\rho}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = $ Liquid phase	697.14 715.33 -18.1 -1346.55 166.12 -67.01	9 69STU/WES	Liquid phas $\Delta_t H^\circ = C_p^\circ =$			2.59	46PRO/JOH
$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = $ Liquid phase $\Delta_t H^{\circ} = S^{\circ} $	697.14 715.33 -18.1 -1346.55 166.12 -67.01	9 69STU/WES	Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ =$		-68.99	2.59	46PRO/JOH
$C_{\rho}^{\circ} = S^{\circ} = S_{\rho}^{\circ} = \Delta_{\rho}S^{\circ} = \Delta_{\rho}G^{\circ} = \ln K_{\ell} = $ Liquid phase	697.14 715.33 -18.1 -1346.55 166.12 -67.01	9 69STU/WES	Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = $		- 68.99 244.38	2.59	46PRO/JOH
$C_{\rho}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = InK_{t} = InK_{t} = InK_{t} = InK_{t}G^{\circ} = InK_{t}G^{$	697.14 715.33 -18.1 -1346.55 166.12 -67.01 -300.00 437.88 667.20	9 69STU/WES	Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ =$		- 68.99 244.38 309.93 - 661.47 128.23	2.59	46PRO/JOH
$C_p^{\circ} = S^{\circ} = S_{\ell}S^{\circ} = \Delta_{\ell}S^{\circ} = \Delta_{\ell}G^{\circ} = \ln K_{\ell} = $ Liquid phase $\Delta_{\ell}H^{\circ} = C_p^{\circ} = $	697.14 715.33 -18.1 -1346.55 166.12 -67.01 -300.00 437.88	9 69STU/WES	Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = $		- 68.99 244.38 309.93 - 661.47	2.59	46PRO/JOH
$C_{\rho}^{\circ} = S^{\circ} = S_{r}^{\circ} = \Delta_{r}S^{\circ} = \Delta_{r}G^{\circ} = InK_{r} = InK_{r}^{\circ} = \Delta_{r}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = InK_{r}^{\circ} = InK_{$	697.14 715.33 -18.1 -1346.55 166.12 -67.01 -300.00 437.88 667.20	9 69STU/WES	Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = $		- 68.99 244.38 309.93 - 661.47 128.23	2.59	46PRO/JOH

(1 × C -(11	$()_{2}(C)(C_{B}))$	< C-(H)(C) ₃) + + (1 × С _в -(C)(($(2 \times -CH_3 \text{ co} C_B)_2) + (5 \times C_1$	rr (tertiary)) + $_{3}$ $-(H)(C_B)_2)$		C_d)(C_B) ₂) + H)(C_B) ₂), σ	$(1 \times C_B - (C)(C_I) = 3$		
	Literature	e – Calculated :	= Residual	Reference	(4 × CB (1	, , -,-,	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ =$	-21.51	- 18.86	-2.65	46PRO/JOH	Gas phase	110.41	117.65	1.54	<00TH 141170
C _p =		174.95			$\Delta_t H^\circ = C_p^\circ = S^\circ =$	118.41 145.18 383.67	116.65 150.36 382.73	1.76 - 5.18 0.94	69STU/WES 69STU/WES 69STU/WES
Liquid phas	e				Δ ₆ S° =		-321.79		
$\Delta_{\rm f}H^{\circ} =$	-69.79	- 69.20	-0.59	46PRO/JOH	$\Delta_{\rm f}G^{\circ} =$		212.59		
$C_{\rho}^{\circ} =$		240.74			$lnK_f =$		– 85.76		
S° =		314.96							
$\Delta_f S^\circ =$		- 656.44			Timela above	_			
$\Delta_f G^\circ =$		126.52			Liquid phase	3	70.50		
$lnK_f =$		-51.04			$\Delta_{\rm f}H^{\circ} =$		70.50 210.28		
			<u> </u>		$C_p^{\circ} = S^{\circ} =$		269.73		
					$\Delta_{f}S^{\circ} =$		- 434.78		
tart Butulba	mana			C10H14	$\Delta_f G^\circ =$		200.13		
tert -Butylbe $(3 \times C - (H)_3)$ $(5 \times C_B - (1)_3)$	(C))+(1×0	$C-(C_B)(C)_3)+($	$(1 \times C_B - (C))(C)$		$\ln K_{\rm f} =$		-80.73		
(**************************************		e – Calculated	= Residual	Reference	meta - Methyl		× C = (B) \ 1 (1	v.C. (H)(C	С,Н,
Gas phase	22.50	- 15.81	-6.78	46PRO/JOH	$(1 \times C_B - (C_B))$		$\times C_{d}-(H)_{2})+(1$ $(1\times C_{B}-(C)(C_{E})$ $= 3$		
$\Delta_{\mathbf{f}}H^{\circ} = C_{p}^{\circ} =$	-22.59	173.27	-0.76	40FKO/JOH		Literatur	e – Calculated :	= Residual	Reference
Liquid phas					Gas phase				
$\Delta_{f}H^{\circ} =$	-70.71	- 64.17	-6.54	46PRO/JOH	$\Delta_t H^\circ -$	115.48	114.76	0.72	69STU/WES
$C_p^{\circ} =$	238.11	238.11	0.00	30HUF/PAR	$C_p^{\circ} =$	145.18	144.67	0.51	69STU/WES
S° =	278.65	278.65	0.00	30HUF/PAR	S° =	389.53	385.23	4.30	69STU/WES
$\Delta_f S^\circ = \Delta_f G^\circ =$		- 692.75 142.37			$\Delta_t S^\circ = \Delta_t G^\circ =$		-319.29 209.96		
$lnK_f =$		-57.43			$lnK_f =$		- 84.69		
Styrene				C ₈ H ₈	Liquid phase	:			
		C_{d} - $(H)(C_{B}))+c$	$(1 \times C_B - (C_d)(0)$	$C_{\rm B})_2)$ +	$\Delta_t H^\circ =$		67.24		
$(5 \times C_B - ($	$(H)(C_B)_2)$, o	= 2			$C_p^{\circ} =$		206.78		
	• • •			5 .	S° =		269.73		
	Literatur	e – Calculated	= Residual	Reference	$\Delta_{f}S^{\circ} =$		-434.78		
					$\Delta_f G^\circ = \ln K_f =$		196.87 79.42		
					mkf -		- 79.42		
Gas nhase	147.82	147.82	0.00	46PIT/GUT		**		***	
Gas phase	1	122.09	0.00	69STU/WES	para-Methyl:	stvrene			C ₉ H ₁₀
$\Delta_i H^{\circ} =$	122.09		-0.10	69STU/WES			$\times C_{d}$ -(H) ₂)+(1	× C ₄ -(H)(C ₂)))+
	122.09 345.10	345.20		. —			$(1 \times C_B - (C)(C_B)$		
$\Delta_f H^\circ = C_p^\circ =$		345.20 223.01			(1 ^ CB-(C	·d八しB/21キ			
$\Delta_{i}H^{\circ} = C_{p}^{\circ} = S^{\circ} =$					$(1 \times C_B - (C_B - (E_B - (E_$				
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$		-223.01			, ,	I)(C _B) ₂), σ		= Residual	Reference
$\Delta_t H^\circ = C_p^o = S^o = S_t S^o = \Delta_t S^o = \ln K_t = $ Liquid phase	345.10	-223.01 214.31 -86.45			(4 × C _B -(1	I)(C _B) ₂), σ	= 6	= Residual	Reference
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phas $\Delta_t H^\circ = S^\circ = \Delta_t H^\circ = S^\circ = S^\circ = \Delta_t H^\circ = S^\circ = S^\circ$	345.10 se 103.47	-223.01 214.31 -86.45	-0.38	45PRO/GIL	(4×C _B -(F	I)(C _B) ₂), σ Literature	= 6 e – Calculated =		
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phas $\Delta_t H^\circ = C_p^\circ =$	345.10 se 103.47 182.88	- 223.01 214.31 - 86.45 103.85 182.88	0.00	46PIT/GUT	$(4 \times C_B - (F_B))$ Gas phase $\Delta_t H^\circ =$	Literature	= 6 e - Calculated =	-0.75	69STU/WES
$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = $ Liquid phas $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = S$	345.10 se 103.47	- 223.01 214.31 - 86.45 103.85 182.88 234.80			$(4 \times C_B - (F_B))^{-1}$ Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = S^\circ = 0$	1)(C _B) ₂), σ Literature 114.64 145.18	= 6 e - Calculated = 115.39 143.96	- 0.75 1.22	69STU/WES 69STU/WES
$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = $ Liquid phas $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t S^{\circ} = \Delta_t S^{\circ} = S^{\circ}$	345.10 se 103.47 182.88	- 223.01 214.31 - 86.45 - 103.85 182.88 234.80 - 333.40	0.00	46PIT/GUT	$(4 \times C_B - (F_B))^{-1}$ Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = S^\circ = 0$	Literature	= 6 e - Calculated =	-0.75	69STU/WES
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{2}$ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \frac{1}{2}$	345.10 se 103.47 182.88	- 223.01 214.31 - 86.45 103.85 182.88 234.80	0.00	46PIT/GUT	$(4 \times C_B - (F_B))$ Gas phase $\Delta_t H^\circ = C_P^\circ =$	1)(C _B) ₂), σ Literature 114.64 145.18	= 6 e - Calculated = 115.39 143.96 379.46	- 0.75 1.22	69STU/WES 69STU/WES

TABLE 11. Aromatic CH-02 (80) - Continued

	$(C_B)_2$ + (1	C_d - $(H)_2$) + $(1 \times C_B$ - $(C)(C_B)_2$)		C ₉ H ₁₀)+	trans-1-Propenylbenzene; trans-β-Methylstyrene $(1 \times C-(H)_3(C)) + (1 \times C_d-(H)(C)) + (1 \times C_d-(H)(C_B)) + (1 \times C_B-(C_d)(C_B)_2) + (5 \times C_B-(H)(C_B)_2), \sigma = 6$				
		- Calculated = R	esidual.	Reference	·	Literatur	e – Calculated =	= Residual	Reference
					Gas phase				
Liquid phase					$\Delta_t H^\circ =$	117.15	115.56	1.59	69STU/WES
$\Delta_t H^\circ =$		67.24			$C_p^{\circ} =$	146.02	145.18	0.84	69STU/WES
$C_p^{\circ} =$		206.78			S° =	380.33	380.91	-0.58	69STU/WES
S° =		269.73			$\Delta_{\mathbf{f}}S^{\circ} =$	000.00	- 323.60	0.00	0,010,1120
$\Delta_{\mathbf{f}}S^{\circ} =$		-434.78			$\Delta_t G^{\circ} =$		212.04		
$\Delta_{\mathbf{f}}G^{\circ} =$		196.87			$\ln K_{\rm f} =$		-85.54		
$lnK_f =$		- 79.42							
	<u> </u>								
					Liquid phas	е			
					$\Delta_{\rm f}H^{\circ} =$		65.54		
Isopropenylber	nzene; α-M	lethylstyrene		C ₉ H ₁₀	$C_p^{\circ} =$		215.59		
		C_{a} -(C)(C_{B})) + (1)+ .:	S° =		260.49		
		$S \times C_B - (H)(C_B)_2$	+		$\Delta_{\mathbf{f}}S^{\circ} =$		- 444.02		
(1×-CH ₃ c	orr (tertiar	y)), $\sigma = 6$			$\Delta_{\mathbf{f}}G^{\circ} =$		197.93		
					$lnK_f =$		<i>−</i> 79.84		
	Literature	– Calculated = R	esidual	Reference	-				
Gas phase					2-Propenylb	enzene			C ₉ H ₁
	112.97	112.97	0.00	69STU/WES			C_d -(H)(C))+(1		(C_B)) +
$C_p^{\circ} = 1$	145.18	145.18	0.00	69STU/WES	$(1 \times C_B - (0))$	$C)(C_B)_2) + (3$	$5 \times C_B - (H)(C_B)$	2)	
-	383.67	383.67	0.00	69STU/WES					
$\Delta_{\rm f}S^{\circ} =$		- 320.84			Lite	erature-Calo	culated = Resid	ual Refere	nce
$\Delta_{\rm f}G^{\circ} =$		208.63							
$lnK_{f} =$		-84.16							
					Liquid phas				
T !! 4 !					$\Delta_{\rm f}H^{\circ}=$	88.03	88.03	0.00	71ROC/MCL
Liquid phase $\Delta_t H^\circ =$	70.46	70.46	0.00	51ROB/JES	-				
$\Delta_{\mathbf{i}}H =$	70.40	70.40	0.00	JIKOB/JES					
					1-Methyl-2-	oronenvlhen	zene		C10H1
							$\times C_{0}$ $-(H)_{2}$ $+ (1)_{2}$	× C.–(H)(C))	
cis-1-Propeny	lbenzene: c	is -B-Methylstyre	ne	C ₉ H ₁₀			$(1 \times -CH_3)$		
(1×C-(H) ₃	$(C)) + (1 \times$	C_{d} -(H)(C))+(1	×cis (unsat)		, ,	/	$5 \times C_B - (H)(C_B)$	` .	,,
				$H)(C_B)_2), \sigma = 6$, - ,		- 、 /、 -/		
$(1 \times C_{d} - (H))$		▼ ∪B=(∪d)(∪B)2)							
					Lite	rature-Cale	culated - Resid	ual Refere	nec
	Literature	- Calculated = R		Reference	Lite	rature-Cak	culated – Reside	ual Refere	nec
	Literature				Liquid phase	e			
Gas phase		– Calculated = R	Residual	Reference	***		56.07	0.00	71ROC/MCL
Gas phase $\Delta_t H^\circ =$	121.34	- Calculated = R	Residual	Reference 69STU/WES	Liquid phase	e			
Gas phase $\Delta_t H^\circ = C_0^\circ =$	121.34 145.18	- Calculated = R 120.41 137.15	0.93 8.03	Reference 69STU/WES 69STU/WES	Liquid phase	e			
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	121.34	- Calculated = R 120.41 137.15 385.97	Residual	Reference 69STU/WES	Liquid phase Δ _t H° –	e 56.07			71ROC/MCL
Gas phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ =$	121.34 145.18	- Calculated = R 120.41 137.15 385.97 - 318.54	0.93 8.03	Reference 69STU/WES 69STU/WES	Liquid phase ΔiII° – Ethynylbenz	e 56.07	56.07	0.00	71ROC/MCL C ₈ H,
Gas phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	121.34 145.18	- Calculated = R 120.41 137.15 385.97 - 318.54 215.38	0.93 8.03	Reference 69STU/WES 69STU/WES	Liquid phase Δ _t II° – Ethynylbenz (1×C _t -(H	e 56.07	56.07 -(C _B)) + (1 × C _I	0.00	71ROC/MCL C ₈ H,
Gas phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ =$	121.34 145.18	- Calculated = R 120.41 137.15 385.97 - 318.54	0.93 8.03	Reference 69STU/WES 69STU/WES	Liquid phase Δ _t II° – Ethynylbenz (1×C _t -(H	e 56.07	56.07 -(C _B)) + (1 × C _I	0.00	71ROC/MCL C ₈ H,
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	121.34 145.18	- Calculated = R 120.41 137.15 385.97 - 318.54 215.38	0.93 8.03	Reference 69STU/WES 69STU/WES	Liquid phase Δ _t II° – Ethynylbenz (1×C _t -(H	e 56.07 H)(1 × C _t + H)(C _B) ₂), σ	56.07 -(C _B)) + (1 × C _I	0.00 s-(C _t)(C _B) ₂) +	71ROC/MCL C ₈ H,
Gas phase $\Delta_t H^\circ = C_\theta^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f =$ Liquid phase	121.34 145.18	- Calculated = R 120.41 137.15 385.97 - 318.54 215.38 - 86.88	0.93 8.03	Reference 69STU/WES 69STU/WES	Liquid phase Δ _t II° – Ethynylbenz (1×C _t -(H	e 56.07 H)(1 × C _t + H)(C _B) ₂), σ	56.07 $-(C_B)) + (1 \times C_I)$ = 2	0.00 s-(C _t)(C _B) ₂) +	71ROC/MCL C ₈ H ₆
Gas phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Lambda_t G^\circ = \ln K_t = $ Liquid phase $\Delta_t H^\circ =$	121.34 145.18	- Calculated = R 120.41 137.15 385.97 - 318.54 215.38 - 86.88	0.93 8.03	Reference 69STU/WES 69STU/WES	Liquid phase ΔμIο – Ethynylbenz (1 × C ₁ -(H (5 × C _B -(H	e 56.07 H)(1 × C _t + H)(C _B) ₂), σ	56.07 $-(C_B)) + (1 \times C_I)$ = 2	0.00 s-(C _t)(C _B) ₂) +	71ROC/MCL C ₈ H ₆
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = $ Liquid phase $\Delta_t H^\circ = C_p^\circ = $	121.34 145.18	- Calculated = R 120.41 137.15 385.97 - 318.54 215.38 - 86.88	0.93 8.03	Reference 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ -$ Ethynylbenz (1×C _t -(H (5×C _B -(I	e 56.07 Sene H)) + $(1 \times C_t$ H) $(C_B)_2$), σ Literature	56.07 $-(C_B)) + (1 \times C_I)$ $= 2$ $= - \text{Calculated} = - \frac{1}{2}$	0.00 $g-(C_1)(C_B)_2) +$ Residual	71ROC/MCL C ₈ H ₄ Reference
Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = S^$	121.34 145.18	- Calculated = R 120.41 137.15 385.97 - 318.54 215.38 - 86.88 70.81 215.59 260.49	0.93 8.03	Reference 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ -$ Ethynylbenz (1×C _t -(H (5×C _B -(I Gas phase $\Delta_t H^\circ =$	e 56.07 Sene H))+(1×C ₁ H)(C _B) ₂), σ Literature	56.07 $-(C_B)) + (1 \times C_I)$ $= 2$ $= -Calculated = 327.48$	0.00 $_{3}-(C_{t})(C_{B})_{2})+$ Residual -0.21	71ROC/MCL C ₈ H ₄ Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \ln K_t = $ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t $	121.34 145.18	- Calculated = R 120.41 137.15 385.97 - 318.54 215.38 - 86.88 70.81 215.59 260.49 - 444.02	0.93 8.03	Reference 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ -$ Ethynylbenz $(1 \times C_t - (H + (5 \times C_B - (H + (1 \times H)^2 + (1 \times H)$	e 56.07 Eene H))+(1×C ₁ H)(C _B) ₂), σ Literature 327.27 114.89	56.07 $-(C_B)) + (1 \times C_B) = 2$ $-(C_B) =$	0.00 a-(C _t)(C _B) ₂) + Residual -0.21 0.00	71ROC/MCL C ₈ H ₄ Reference 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = $	121.34 145.18	- Calculated = R 120.41 137.15 385.97 - 318.54 215.38 - 86.88 70.81 215.59 260.49 - 444.02 203.20	0.93 8.03	Reference 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ -$ Ethynylbenz $(1 \times C_t - (H + (5 \times C_B - (H + (1 \times H)^2 + (1 \times H)^2 + (1 \times H)^2)))$ Gas phase $\Delta_t H^\circ =$ $C_t^\circ =$ $S^\circ =$	e 56.07 Sene H))+(1×C ₁ H)(C _B) ₂), σ Literature	56.07 $-(C_B)) + (1 \times C_B) = 2$ $-(C_B) + (C_B) = 2$ $-($	0.00 $_{3}-(C_{t})(C_{B})_{2})+$ Residual -0.21	71ROC/MCL C ₈ H ₄ Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \ln K_t = $ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t $	121.34 145.18	- Calculated = R 120.41 137.15 385.97 - 318.54 215.38 - 86.88 70.81 215.59 260.49 - 444.02	0.93 8.03	Reference 69STU/WES 69STU/WES	Liquid phase $\Delta_t II^\circ -$ Ethynylbenz $(1 \times C_t - (H + (5 \times C_B - (H + (1 \times C_t)))))$ Gas phase $\Delta_t H^\circ = C_t^\circ = C_$	e 56.07 Eene H))+(1×C ₁ H)(C _B) ₂), σ Literature 327.27 114.89	56.07 -(C _B)) + (1 × C _I = 2 e - Calculated = 327.48 114.89 321.67 -115.97	0.00 a-(C _t)(C _B) ₂) + Residual -0.21 0.00	71ROC/MCL C ₈ H ₄ Reference 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = $	121.34 145.18	- Calculated = R 120.41 137.15 385.97 - 318.54 215.38 - 86.88 70.81 215.59 260.49 - 444.02 203.20	0.93 8.03	Reference 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ -$ Ethynylbenz $(1 \times C_t - (H + (5 \times C_B - (H + (1 \times H)^2 + (1 \times H)^2 + (1 \times H)^2)))$ Gas phase $\Delta_t H^\circ =$ $C_t^\circ =$ $S^\circ =$	e 56.07 Eene H))+(1×C ₁ H)(C _B) ₂), σ Literature 327.27 114.89	56.07 $-(C_B)) + (1 \times C_B) = 2$ $-(C_B) + (C_B) = 2$ $-($	0.00 a-(C _t)(C _B) ₂) + Residual -0.21 0.00	71ROC/MCL C ₈ H ₄ Reference 69STU/WES 69STU/WES

TABLE 11.	Aromatic	CH-02	(80)	- Co	ntinued
IABLE II.	AIGHIAGC	CH-02	LOUI	- 0	munucu

Table 11.	Aromatic CH-02	(80)	_	Continued
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		$-(C_B)$) + (1 × C	$C_B - (C_t)(C_B)_2$	C ₈ H ₆		$H_{3}(C)) + (4$	nethane $S \times C_B - (C)(C_B)_2$ $(1 \times ortho \text{ corr})$		
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid phase Δ _t H° =	282.88	283.39	-0.51	58FLI/SKI	Gas phase $\Delta_t H^\circ =$	و المالية الم	74.09	- 17 - 18	
Diphenylmet (1×C-(H	$)_2(C_B)_2)+($	2×C _B -(C)(C _B e – Calculated		$C_{13}H_{12}$ $-(H)(C_B)_2)$ Reference	Liquid pha $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \Delta_t G^\circ = C_p^\circ = C_$	se 24.69	23.46 331.21 371.53 -759.14 249.80	1.23	76GOO/LEE
Gas phase $\Delta_t H^\circ =$	138.95	138.95	0.00	59AIH	$lnK_f =$		-100.77		
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	89.66 279.91 301.67	93.42 279.91 301.67 - 556.38 259.30 - 104.60	-3.76 0.00 0.00	50PAR/MOS2 50KUR 30HUF/PAR	(1×−CH (10×C _B -	$H_{3}(C)$) + (1 $H_{3}(C)$)	\times C-(H)(C)(C ₁ iary)) + (2 \times C ₂ - lculated = Resid	-(C)(C _B) ₂)+	C ₁₄ H ₁₄
Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	71.09 223.84 239.32	71.66 223.84 239.35 -618.70 256.12 -103.32	-0.57 0.00 -0.03	30HUF/PAR 30HUF/PAR 30HUF/PAR	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} =$	48.66 294.97	48.66 294.98 361.12 -633.24 237.46 -95.79	0.00 -0.01	53COO/MUL 31SMI/AND
4-Methyldipi (1×C-(H (1×C-(H	(C)) + (3) (C_B) 2)	$\times C_B - (C)(C_B)_2$		C ₁₄ H ₁₄)(C _B) ₂) +	$(2 \times C_{B}-($	$(1)_3(C) + (1)_3(C)(C_B)_2 + (1)_3(C)$	$0 \times C - (H)_2(C)_2$ $(10 \times C_B - (H)(C)$ $ culated = Resid$	в)2)	
Gas phase Δ _i H° =	Literatur	e – Calculated	= Residual	Reference	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	593.71 684.92	- 206.46 599.18 684.92 - 1672.55	-5.47 0.00	60KAR/STR2 60KAR/STR2
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	61.55	56.81 303.81 336.60 -657.76 252.92 -102.03	4.74	76GOO/LEE	$\Delta_f G^\circ = \ln K_f = $ $1,1-Dipheny$ $(1 \times C_d - (1 + 1))$		$\begin{array}{c} 292.21 \\ -117.88 \end{array}$ $C_{d} - (C_{B})_{2}) + (2 \times C_{B})_{2} + (2 \times C_{B})_{2}$	C_{B} – $(C_{d})(C_{B})$	C ₁₄ H ₁₂
						Literatur	e – Calculated =	= Residual	Reference
					Gas phase $\Delta_f H^\circ =$	245.64	245.64	0.00	56HOL/TYR

TABLE 11. Aromatic CH-02 (80) - Continued

(10×C _B -(e – Calculated :	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
					0 1				
iquid phase \ _t H° =	e 172.42	172.42	0.00	50COO/HOI	Gas phase $\Delta_t H^\circ =$	142.93	142.70	0.23	59AIH
$C_p^{\circ} =$	299.16	299.15	0.01	31SMI/AND	$C_p^{\circ} =$	1,2,33	206.82	0.20	<i>37</i> 1111
					Liquid phas	e			
s-Stilbene				C ₁₄ H ₁₂	$\Delta_{\rm f}H^{\circ} =$		70.30		
		$\times C_B - (C_d)(C_B)$	$)_2) + (10 \times C_{B}$	$-(H)(C_B)_2) +$	$C_p^{\circ} =$		292.80		
(1×cis(ui	nsat) corr)				$S^{\circ} = \Delta_t S^{\circ} =$		344.50 - 649.86		
	Literature	c — Calculated	- Residual	Reference	$\Delta_{i}G^{\circ} =$		264.05		
					$lnK_f =$		-106.52		
Gas phase					·				
$\Delta_{\rm f}H^{\circ} =$	252.55	247.85	4.70	52BRA/PLE	Solid phase				
$C_{\rho}^{\circ} =$		193.39			$\Delta_t H^\circ =$	51.51	48.90	2.61	66COL/PIL
					$C_p^{\circ} =$	253.55	253.54	0.01	31SMI/AND
!!.db	_				$S^{\circ} = \Delta_{t}S^{\circ} =$	270.29	270.30	- 0.01	30HUF/PAR
Liquid phas Δ _t H° =	e 183.51	169.47	14.04	50COO/HOI	$\Delta_{\mathbf{f}} S^{\circ} = \Delta_{\mathbf{f}} G^{\circ} =$		- 724.06 264.78		
$C_p^{\circ} =$	103.31	309.02	14.04	SUCCOO/HOI	$\ln K_{\rm f} =$		- 106.81		
$S^{\circ} =$		297.22			mrt -		-100.61		
$\Delta_{f}S^{*} =$		- 566.57							
		338.39							
Δ _f G =		220.27							
$\ln K_f =$		-136.50			Triphenylmo				C ₁₉ H
	1						$3 \times C_B - (C)(C_B)$	$_2) + (15 \times C_B - ($	
$lnK_f =$	ne			CuHu		$)(C_B)_3)+(3$	$3 \times C_B - (C)(C_B)$ re – Calculated		
$lnK_{f} =$) ₂)+(10×C _B ·	C ₁₄ H ₁₂ -(H)(C _B) ₂)	(1×C-(H	$)(C_B)_3)+(3$			$(H)(C_B)_2)$
trans -Stilbe	H)(C_B)) + (2	- 136.50				$)(C_B)_3)+(3$			$(H)(C_B)_2)$
$lnK_f =$ trans-Stilber $(2 \times C_d - (1))$	H)(C_B)) + (2	-136.50 2×C _B -(C _d)(C _B		-(H)(C _B) ₂)	Gas phase Δ _t H° =	$)(C_B)_3)+(3$	e – Calculated		$(H)(C_B)_2)$
$lnK_f =$ rans-Stilber $(2 \times C_d - (1))$ Gas phase	H)(C _B)) + (2	-136.50 $2 \times C_B - (C_d)(C_B$ $e - Calculated$		-(H)(C _B) ₂)	Gas phase $\Delta_t H^\circ =$ Solid phase	$)(C_B)_3)+(3$	e – Calculated		$(H)(C_B)_2)$
$lnK_f =$	H)(C_B)) + (2	-136.50 2×C _B -(C _d)(C _B	= Residual	-(H)(C _B) ₂) Reference	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$	$)(C_B)_3)+(3$	e – Calculated		$(H)(C_B)_2)$
$lnK_f =$ rans-Stilber $(2 \times C_d - (1))$ Gas phase	H)(C _B)) + (2	-136.50 $2 \times C_{B} - (C_{d})(C_{B}$ $e - Calculated$ 243.00	= Residual	-(H)(C _B) ₂) Reference	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_t^\circ =$ $S_t^\circ =$)(C _B) ₃) + (2	271.21 174.13	= Residual	(H)(C _B) ₂) Reference
In K_f = rans-Stilbe $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p^\circ = C_p^\circ = C_p^\circ = C_p^\circ$	H)(C _B)) + (2 Literatur 239.70	-136.50 $2 \times C_{B} - (C_{d})(C_{B}$ $e - Calculated$ 243.00	= Residual	-(H)(C _B) ₂) Reference	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$)(C _B) ₃) + (2 Literatur 295.39	271.21 174.13 295.81 312.13 -841.50	= Residual	(H)(C _B) ₂) Reference 31SMI/AND
In K_f = rans-Stilber $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase	H)(C _B)) + (2 Literatur 239.70	-136.50 2 × C _B -(C _d)(C _B e - Calculated 243.00 201.42	= Residual	-(H)(C _B) ₂) Reference	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_t^\circ =$ $S_t^\circ =$ $\Delta_t S_t^\circ =$ $\Delta_t G_t^\circ =$)(C _B) ₃) + (2 Literatur 295.39	271.21 174.13 295.81 312.13 -841.50 425.02	= Residual	(H)(C _B) ₂) Reference 31SMI/AND
In K_f = rans-Stilber $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p$	H)(C _B)) + (2 Literatur 239.70	-136.50 2 × C _B -(C _d)(C _B e - Calculated 243.00 201.42	= Residual	-(H)(C _B) ₂) Reference	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$)(C _B) ₃) + (2 Literatur 295.39	271.21 174.13 295.81 312.13 -841.50	= Residual	(H)(C _B) ₂) Reference 31SMI/AND
In K_f = Trans-Stilber $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_$	H)(C _B)) + (2 Literatur 239.70	-136.50 2 × C _B -(C _d)(C _B e - Calculated 243.00 201.42 164.20 309.02	= Residual	-(H)(C _B) ₂) Reference	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_t^\circ =$ $S_t^\circ =$ $\Delta_t S_t^\circ =$ $\Delta_t G_t^\circ =$)(C _B) ₃) + (2 Literatur 295.39	271.21 174.13 295.81 312.13 -841.50 425.02	= Residual	(H)(C _B) ₂) Reference 31SMI/AND
In K_f = rans-Stilbe: $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	H)(C _B)) + (2 Literatur 239.70	-136.50 2 × C _B -(C _d)(C _B e - Calculated 243.00 201.42 164.20 309.02 297.22	= Residual	-(H)(C _B) ₂) Reference	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_t^\circ =$ $S_t^\circ =$ $\Delta_t S_t^\circ =$ $\Delta_t G_t^\circ =$)(C _B) ₃) + (2 Literatur 295.39	271.21 174.13 295.81 312.13 -841.50 425.02	= Residual	(H)(C _B) ₂) Reference 31SMI/AND
In K_f = Trans-Stilber (2 × C _d -(1) Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ $S^\circ = \Delta_t S^\circ =$	H)(C _B)) + (2 Literatur 239.70	-136.50 2 × C _B -(C _d)(C _B e - Calculated 243.00 201.42 164.20 309.02 297.22 -566.57	= Residual	-(H)(C _B) ₂) Reference	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $S^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t =$	295.39 312.13	271.21 174.13 295.81 312.13 -841.50 425.02	= Residual	Reference 31SMI/AND 30HUF/PAR
In K_f = rans-Stilbe: $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ =$ $\Delta_t G^\circ =$	H)(C _B)) + (2 Literatur 239.70	-136.50 2×C _B -(C _d)(C _B e - Calculated 243.00 201.42 164.20 309.02 297.22 -566.57 333.12	= Residual	-(H)(C _B) ₂) Reference	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t =$ Tetraphenyl	295.39 312.13	271.21 174.13 295.81 312.13 -841.50 425.02 -171.45	= Residual -0.42 0.00	(H)(C _B) ₂) Reference 31SMI/AND 30HUF/PAR
In K_f = rans-Stilber $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$ $\Delta_t S^\circ =$	H)(C _B)) + (2 Literatur 239.70	-136.50 2 × C _B -(C _d)(C _B e - Calculated 243.00 201.42 164.20 309.02 297.22 -566.57	= Residual	-(H)(C _B) ₂) Reference	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t =$ Tetraphenyl	295.39 312.13	271.21 174.13 295.81 312.13 -841.50 425.02 -171.45 C _B -(C)(C _B) ₂)+	= Residual - 0.42 0.00	(H)(C _B) ₂) Reference 31SMI/AND 30HUF/PAR C ₂₅ H
In K_f = rans-Stilbe: $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p$	H)(C _B)) + (2 Literatur 239.70	-136.50 2 × C _B -(C _d)(C _B e - Calculated 243.00 201.42 164.20 309.02 297.22 -566.57 333.12 -134.38	= Residual	-(H)(C _B) ₂) Reference 72MOR2	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t =$ Tetraphenyl	295.39 312.13	271.21 174.13 295.81 312.13 -841.50 425.02 -171.45	= Residual - 0.42 0.00	(H)(C _B) ₂) Reference 31SMI/AND 30HUF/PAR
In K_f = rans-Stilber $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p$	H)(C _B)) + (2 Literatur 239.70 se	-136.50 2 × C _B -(C _d)(C _B e - Calculated 243.00 201.42 164.20 309.02 297.22 -566.57 333.12 -134.38	= Residual - 3.30	Teference 72MOR2 50COO/HOI	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_t^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Tetraphenyl $(1 \times C - (C_t^*)^{-1} \times C - (C_t^*)^{-1}$	295.39 312.13	271.21 174.13 295.81 312.13 -841.50 425.02 -171.45 C _B -(C)(C _B) ₂)+	= Residual - 0.42 0.00	(H)(C _B) ₂) Reference 31SMI/AND 30HUF/PAR C ₂₅ H
In K_f = rans-Stilbe $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p^$	H)(C _B)) + (2 Literatur 239.70 See 140.50 232.60	-136.50 2 × C _B -(C _d)(C _B e - Calculated 243.00 201.42 164.20 309.02 297.22 -566.57 333.12 -134.38	- 3.30 - 0.40 0.00	Teference 72MOR2 50COO/HOI 31SMI/AND	Gas phase $\Delta_t H^\circ = {C_r^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = {1 \times C_r^\circ (C_t^\circ = C_t^\circ = C_t$	295.39 312.13	271.21 174.13 295.81 312.13 -841.50 425.02 -171.45 C _B -(C)(C _B) ₂)+ e-Calculated	= Residual - 0.42 0.00	(H)(C _B) ₂) Reference 31SMI/AND 30HUF/PAR C ₂₅ F
In K_f = rans-Stilber $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p$	H)(C _B)) + (2 Literatur 239.70 se	-136.50 2 × C _B -(C _d)(C _B e - Calculated 243.00 201.42 164.20 309.02 297.22 -566.57 333.12 -134.38 140.90 232.60 251.00	= Residual - 3.30	Teference 72MOR2 50COO/HOI	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_t^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Tetraphenyl $(1 \times C - (C_t^*)^{-1} \times C - (C_t^*)^{-1}$	295.39 312.13	271.21 174.13 295.81 312.13 -841.50 425.02 -171.45	= Residual - 0.42 0.00	(H)(C _B) ₂) Reference 31SMI/AND 30HUF/PAR C ₂₅ I
In K_f = rans-Stilber $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p$	H)(C _B)) + (2 Literatur 239.70 See 140.50 232.60	-136.50 2 × C _B -(C _d)(C _B e - Calculated 243.00 201.42 164.20 309.02 297.22 -566.57 333.12 -134.38 140.90 232.60 251.00 -612.79	- 3.30 - 0.40 0.00	Teference 72MOR2 50COO/HOI 31SMI/AND	Gas phase $\Delta_t H^\circ = {C_r^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = {1 \times C_r^\circ (C_t^\circ = C_t^\circ = C_t$	295.39 312.13	271.21 174.13 295.81 312.13 -841.50 425.02 -171.45 C _B -(C)(C _B) ₂)+ e-Calculated	= Residual - 0.42 0.00	(H)(C _B) ₂) Reference 31SMI/AND 30HUF/PAR C ₂₅ I
In K_f = rans-Stilber $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ = $ $\Delta_t H^\circ = C_p^\circ = $ $\Delta_t S^\circ = \Delta_t S^\circ = $ $\Delta_t H^\circ = C_p^\circ = $ Solid phase $\Delta_t H^\circ = C_p^\circ = $ $S^\circ = \Delta_t S^\circ = $ $\Delta_t S^\circ = \Delta_t S^\circ = $ $\Delta_t S^\circ = $ $\Delta_t S^\circ = $	H)(C _B)) + (2 Literatur 239.70 See 140.50 232.60	-136.50 2×C _B -(C _d)(C _B e - Calculated 243.00 201.42 164.20 309.02 297.22 -566.57 333.12 -134.38 140.90 232.60 251.00 -612.79 323.60	- 3.30 - 0.40 0.00	Teference 72MOR2 50COO/HOI 31SMI/AND	Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S_p^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t =$ Tetraphenyl $(1 \times C - (C))$ Gas phase $\Delta_t H^\circ =$	295.39 312.13	271.21 174.13 295.81 312.13 -841.50 425.02 -171.45 C _B -(C)(C _B) ₂)+ e-Calculated	= Residual - 0.42 0.00	(H)(C _B) ₂) Reference 31SMI/AND 30HUF/PAR C ₂₅ I
In K_f = rans-Stilber $(2 \times C_d - (1))$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p$	H)(C _B)) + (2 Literatur 239.70 See 140.50 232.60	-136.50 2 × C _B -(C _d)(C _B e - Calculated 243.00 201.42 164.20 309.02 297.22 -566.57 333.12 -134.38 140.90 232.60 251.00 -612.79	- 3.30 - 0.40 0.00	Teference 72MOR2 50COO/HOI 31SMI/AND	Gas phase $\Delta_t H^\circ = {C_r^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = {1 \times C_r^\circ (C_t^\circ = C_t^\circ = C_t$	295.39 312.13	271.21 174.13 295.81 312.13 -841.50 425.02 -171.45 C _B -(C)(C _B) ₂)+ e-Calculated	= Residual - 0.42 0.00	(H)(C _B) ₂) Reference 31SMI/AND 30HUF/PAR (C ₂₅ I

TABLE 11. Aromatic CH-02 (80) — Continued	TABLE 11.	Aromatic	CH-02 (80) -	Continued
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TABLE 11. Aromatic CH-02 (80) - Continued

$\label{eq:control_loss} \begin{array}{ll} \textbf{1,1,2-Triphenylethane} & C_{20}H_{18} \\ (1\times C-(H)_2(C)(C_B)) + (1\times C-(H)(C)(C_B)_2) + (3\times C_B-(C)(C_B)_2) + \\ (15\times C_B-(H)(C_B)_2) & \end{array}$	$(1 \times C - (C_B)_3(C)) + (1 \times C - (H)(C)(C_B)_2) + (5 \times C_B - (C)(C_B)_2) + (25 \times C_B - (H)(C_B)_2)$				
Literature-Calculated = Residual Reference	Literature-Calculated = Residual Reference				
Liquid phase $\Delta_t H^{\circ} = 133.60$ $C_p^{\circ} = 404.90$ $S^{\circ} = 450.07$	Solid phase $\Delta_t H^\circ = 365.40$ $C_\rho^\circ = 473.63 470.33 3.30 31SMI/AN$	1D			
$ \Delta_{i}S^{\circ} = -839.87 $ $ \Delta_{f}G^{\circ} = 384.01 $ $ inK_{f} = -154.91 $	$\label{eq:continuous} \begin{split} \text{Triphenylethylene} & C \\ & (1 \times C_d - (C_B)_2) + (1 \times C_d - (H)(C_B)) + (3 \times C_B - (C_d)(C_B)_2) + \\ & (15 \times C_B - (H)(C_B)_2) \end{split}$	H₁			
Solid phase $\Delta_t H^\circ = 133.95$	Literature – Calculated = Residual Reference				
$C_p^{\circ} = 319.66 325.10 -5.44 31SMI/AND$	Gas phase $\Delta_t H^\circ = 340.82$				
$\label{eq:continuous} \begin{array}{ll} \textbf{1,1,1-Triphenylethane} & C_{20}H_{18} \\ (1\times C-(H)_3(C))+(1\times C-(C_B)_3(C))+(1\times -CH_3 \text{ corr (tertiary)})+\\ (3\times C_B-(C)(C_B)_2)+(15\times C_B-(H)(C_B)_2) \\ \\ \text{Literature-Calculated} = Residual & Reference \\ \end{array}$	Liquid phase $\Delta_l H^{\circ} = 232.77$ $C_p^{\circ} = 425.29$				
Solid phase $\Delta_t H^\circ = 206.82$ $C_p^\circ = 316.73$ 339.45 -22.72 31SMI/AND	Solid phase $\Delta_l H^\circ = 233.38$ 226.20 7.18 50COO/HC $C_P^\circ = 309.20$ 310.10 -0.90 31SMI/AN				
1,1,1,2-Tetraphenylethane $ \begin{array}{c} C_{26}H_{22} \\ (1\times C-(C_B)_3(C)) + (1\times C-(H)_2(C)(C_B)) + (4\times C_B-(C)(C_B)_2) + \\ (20\times C_B-(H)(C_B)_2) \end{array} $	Diphenylacetylene $(2 \times C_t - (C_B)) + (2 \times C_B - (C_t)(C_B)_2) + (10 \times C_B - (H)(C_B)_2)$ Literature – Calculated = Residual Reference	14H 10			
Literature-Calculated = Residual Reference	Gas phase $\Delta_t H^\circ = 427.96$				
Solid phase $\Delta_t H^\circ = 280.35$ $C_p^\circ = 395.39$ 398.77 -3.38 31SMI/AND	$C_p^o =$ 184.68 Liquid phase $\Delta_i H^o =$ 357.84				
1,1,2,2-Tetraphenylethane $ C_{2e}H_{22} $ $ (2 \times C-(H)(C)(C_B)_2) + (4 \times C_B-(C)(C_B)_2) + (20 \times C_B-(H)(C_B)_2) $ $ Literature-Calculated = Residual \qquad Reference $	Solid phase $\Delta_t H^\circ = 312.40 312.00 0.40 53\text{COO/HC}$ $C_p^\circ = 225.90 225.90 0.00 31\text{SMI/ANI}$	-			
Liquid phase $\Delta_t H^{\circ} = 196.90$	Biphenyl $(2 \times C_B - (C_B)_3) + (10 \times C_B - (H)(C_B)_2), \ \sigma = 8$	₁₂ H ₁₀			
$C_p^{\circ} = 517.00$ $S^{\circ} = 555.64$ $\Delta_p S^{\circ} = -1029.88$	Literature - Calculated = Residual Reference				
$\Delta_t G^\circ = 503.96$ $\ln K_t = -203.29$ Solid phase $\Delta_t H^\circ = 219.00$	Gas phase $\Delta_i H^\circ = 182.03$ 181.42 0.61 89CHI/KNI $C_p^\circ = 162.34$ 162.34 0.00 69STU/WE. $S^\circ = 392.67$ 392.67 0.00 69STU/WE. $\Delta_i S^\circ = -329.06$ $\Delta_i G^\circ = 279.53$	S			
$C_p^{\circ} = 396.64 396.66 -0.02 31\text{SMI/AND}$	$\ln K_f = 279.33$ $\ln K_f = -112.76$				

TABLE 11. Aromatic CH-02 (80) - Continued

TABLE 11.	Aromatic	CH-02 (80) -	Continued
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Biphenyl (Co (2×C _B –(C	ontinued) $C_{\rm B})_3) + (10 \times$	$C_B-(H)(C_B)_2$, σ = 8	$C_{12}H_{10}$		3(C))+(1×	$C_B-(C)(C_B)_2$	+(1×ortho	C ₁₃ H ₁₂ corr)+
	Literature	- Calculated =	= Residual	Reference	$(2\times C_B-(C_B)$	в)3) + (9×С	$_{\rm B}$ -(H)(C _B) ₂)		
						Literature	Calculated -	- Residual	Reference
Liquid phase		444.00	2.10	006777					
$\Delta_{f}H^{\circ} = C_{p}^{\circ} =$	119.12	116.02 260.94	3.10	89CHI/KNI	Liquid phase $\Delta_t H^\circ = C_p^\circ =$	108.16	82.67 288.34	25.49	35BRU
Solid phase								·	
$\Delta_{\mathbf{f}}H^{\circ} =$	100.54	99.36	1.18	66COL/PIL					
$C_p^{\circ} =$	198.39	197.86	0.53	89CHI/KNI	3-Methylbiph				C ₁₃ H ₁₂
S° =	209.38	215.50	-6.12	89CHI/KNI	$(1 \times C - (H))$	3(C))+(1×	C_B – $(C)(C_B)_2)$	+(1×meta c	orr)+
$\Delta_f S^\circ =$		-506.23			$(2\times C_B-(C_B)$	в)3) + (9 × C	$_{\rm B}$ - $(H)(C_{\rm B})_2)$		
$\Delta_f G^\circ = \ln K_f =$		250.29 100.97				T	01.1.1		D (
		100.57				Literature	- Calculated =	= Residual	Reference
					Gas phase				
Naphthalen	е			$C_{10}H_{8}$	$\Delta_t H^\circ =$		148.36		
	(C _{BF})(C _B) ₂) thalene 0 si	$+(8\times C_B-(H)($	$(C_B)_2) +$		$C_p^{\circ} =$		184.92		
(= - : ::=p:::		e – Calculated :	= Residual	Reference	Timil above				
	Littiatui	e Calculateu -	- Residuai	Reference	Liquid phase	05.50	70.41	C 15	250011
					$\Delta_{\rm f}H^{\circ} = C_{\rm p}^{\circ} =$	85.56	79.41 284.84	6.15	35BRU
Gas phase					$C_p =$		204.04		
$\Delta_{\rm f} H^{\circ} =$	150.63	150.68	-0.05	63MIL					
$C_p^{\circ} =$	132.55	132.54	0.01	69STU/WES					
S° =	335.64	335.63	0.01	69STU/WES	4-Methylbiph	envl			C13H12
$\Delta_f S^{\circ} =$		- 244.05					$C_B-(C)(C_B)_2$	$+(2\times C_{B}-(C_{I}))$	
$\Delta_t G^{\circ} =$		223.44			(9×C _B -(H		-5 (-)(-5/2)	(= 1 - 5 (-)	D)3)
$lnK_f =$		- 90.14				, , ,,,,	Calantatada	Dealdool	D
						Literature -	- Calculated =	= Residuai	Reference
Liquid phas		06.04	0.07	ETN ACCURENT					
$\Delta_t H^\circ =$	95.97	96.94	-0.97	57MCC/FIN	Gas phase				
$C_{\rho}^{\circ} = S^{\circ} =$		200.48 219.88			$\Delta_t H^\circ =$		148.99		
3 = Δ _f S° =		359.80			$C_p^{\circ} =$		184.21		
$\Delta_{\rm f}G^{\circ} =$		204.22			***				
$\ln K_{\rm f} =$		-82.38			T !! 1!				
maxi —		02.50			Liquid phase $\Delta_t H^\circ =$		79.41		
					$C_p^{\circ} =$		284.84		
Solid phase					C_p –		204.04		
$\Delta_{f}H^{\circ} =$	77.74	80.44	-2.70	66COL/PIL					
$C_p^{\circ} =$	165.69	165.64	0.05	57MCC/FIN	Solid phase				
s° =	167.40	170.00	-2.60	57MCC/FIN	$\Delta_t H^\circ =$	55.44	59.99	-4.55	35BRU
$\Delta_{\mathbf{f}}S^{\circ} =$		-409.68			$C_p^{\circ} =$	33.44	221.92	4.00	SSERC
$\Delta_{\rm f}G^{\circ} =$		202.59			$S^a =$		243.94		
$lnK_f =$		-81.72			$\Delta_{\mathbf{f}}S^{\circ} =$		-614.11		
					$\Delta_t G^{\circ} =$		243.09		
					$lnK_f =$		- 98.06		
	•					··-	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		
2-Methylbir				C ₁₃ H ₁₂	-				
		$\times C_B - (C)(C_B)_2$ $C_B - (H)(C_B)_2$	+ (1×ortho	corr)+					
		e – Calculated	= Residual	Reference					
Gas phase									
Gas phase $\Delta_i H^\circ = C_p^\circ =$	- Ditorutur	150.25 190.61							

TABLE 11	Aromatic	CH-02	(80) -	Continued
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- Continued TABLE 11. Aromatic CH-02 (80) - Continued

	$(1)_3(C) + (1)$	< C−(H)(C) ₂ (C ury)) + (1 × C _B -		C ₁₅ H ₁₆	ortho-Terph (4×C _B -(•	$< C_B - (H)(C_B)_2$)	C ₁₈ H ₁ ,
	corr) + (9×	$C_B-(H)(C_B)_2$ C_B -Calculated	$+(2\times C_B-(C_1)$			Literatur	e – Calculated	= Residual	Reference
	Literature			Reference	Gas phase				
Gas phase $\Delta_t H^\circ = C_p^\circ =$		98.95 238.79			$\Delta_t H^\circ = C_\rho^\circ =$		279.98 243.02		
Liquid phas	e	04.00			Liquid phas $ \Delta_t H^\circ = C_p^\circ = $	e	183.08 385.80		
$\Delta_t H^\circ = C_p^\circ =$	338.49	24.88 342.32	-3.83	64VUK/RAS	<u> </u>				,
	l) ₃ (C))+(1: thalene 1 su	\times C _B -(C)(C _B) ₂ ub) + (7 \times C _B -(e - Calculated	$H)(C_B)_2), \sigma =$		Solid phase $ \Delta_t H^\circ = \\ C_p^\circ = \\ S^\circ - \\ \Delta_t S^\circ = \\ \Delta_t G^\circ = \\ \ln K_t = $	274.34 298.82	159.54 274.94 294.50 722.82 375.05 151.29	- 0.60 4.32	72CHA/BES 72CHA/BES
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	116.86 159.54 377.44	118.25 159.53 377.75	-1.39 0.01 -0.31	69STU/WES 69STU/WES 69STU/WES	1,3,5-Triphe	-)	С24Н11
$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-338.25 219.10 -88.38				Literatur	e – Calculated	= Residual	Reference
Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = A_s S^\circ $	56.19 224.39 254.81	60.33 224.38 254.81	-4.14 0.01 0.00	60SPE/ROS 57MCC/FIN 57MCC/FIN	Gas phase $\Delta_t H^\circ = C_p^\circ =$		378.54 323.70		
$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$		-461.18 197.83 -79.80			Liquid phas $\Delta_t H^\circ = C_p^\circ =$	e	250.14 510.66		
4,4'-Dimeth (2×C-(F (8×C _B -(I) ₃ (C)) + (2: H)(C _B) ₂)	$\times C_B$ -(C)(C_B) ₂ $= - Calculated$		C ₁₄ H ₁₄ B)3) + Reference	Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	358.32 367.36	219.72 352.02 373.50 - 939.40 499.80	6.30 -6.14	36PAR/TOD 36PAR/TOD
Gas phase $\Delta_t H^\circ = C_p^\circ =$		116.56 206.08			$lnK_f =$		-201.62		
Liquid phas $\Delta_l H^\circ = C_l^\circ =$	e	42.80 308.74			2-Methylnap (1×C-(H (2×napht) ₃ (C))+(1> halene 1 su	$(C_B-(C)(C_B)_2)$ b) + $(7 \times C_B-(1)$ c - Calculated =	$H)(C_B)_2), \sigma =$	$C_{11}H_{10}$ C_{BF})(C_{B}) ₂) + C_{BF} 3 Reference
Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	14.14	20.62 245.98 272.38 - 721.98 235.88 - 95.15	-6.48	35BRU	Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	116.11 159.79 380.03	118.25 159.53 377.75 - 338.25 219.10 - 88.38	-2.14 0.26 2.28	69STU/WES 69STU/WES 69STU/WES

TABLE 11. Aromatic CH-02 (80) - Continued

	3(C))+(1: nalene 1 si	$\times C_{B}-(C)(C_{B})_{2})$ $ub) + (7 \times C_{B}-(I_{B})$	$H)(C_B)_2), \sigma =$: 3	$(1 \times C - (I \times C) + (1 \times C))$		\times C-(H) ₂ (C)(C +(2 × naphtha		
i	Literatur	e – Calculated =	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Liquid phase		60.00	2.25	car rocativi	T111.1				
$\Delta_{\rm f}H^{\circ} = C^{\circ} - V^{\circ}$	62.58	60.33	2.25	57MCC/FIN	Liquid pha	se	25 52		
$C_p^\circ = {}^{\circ} \cdot {}^{\circ}$ $S^\circ = {}^{\circ} \cdot {}^{\circ}$		224.38 254.81			$\Delta_t H^\circ = C_p^\circ =$		35.52 247.28		
Δ _f S° =		-461.18			$S^{\circ} =$		302.21		
∆್.G° =		197.83			$\Delta_f S^\circ =$		-550.10		
$\ln K_t =$		- 79.80			$\Delta_{\mathbf{f}}G^{\circ} =$		199.53		
					$\ln K_{\rm f} =$		- 80.49		
olid phase									
$\Delta_{\mathbf{f}}H^{\circ} =$	44.85	41.07	3.78	60SPE/ROS	1-Propylna				C ₁₃ l
$C_p^{\circ} =$	195.98	189.70	6.28	57MCC/FIN	(1×C-(H	(C) + (1)	\times C-(H) ₂ (C) ₂)	$+(1\times C-(H)_2$	$(C)(C_B)) +$
S° =	219.99	198.44	21.55	57MCC/FIN	$(1 \times C_{B}-($	$C)(C_B)_2)+($	$2 \times C_{BF} - (C_{BF})($	$(C_B)_2) +$	
$\Delta_{\rm r} S^{\circ} =$		-517.55			(2×naph	thalene 1 si	$ab) + (7 \times C_B - (1)$	$H)(C_B)_2), \sigma =$	= 3
$\Delta_{\mathbf{f}}G^{\circ} = $ $\ln K_{\mathbf{f}} =$		195.38 78.81				Literatur	e – Calculated :	= Residual	Reference
······································					<u></u>				
-Ethylnapht	thalene			$C_{12}H_{12}$	Gas phase				
		\times C-(H) ₂ (C)(C		$(C)(C_B)_2) +$	$\Delta_{\rm f}H^{\circ} =$	74.68	76.28	-1.60	69STU/WES
) + (2×naphtha	lene 1 sub)+		$C_p^{\circ} =$	208.11	208.03	0.08	69STU/WES
$(7 \times C_{B} - (11))$	I)(С _в) ₂), а	r - 3			S° =	158.36	459.50	- 1.14	69STU/WES
					$\Delta_{\mathbf{f}}S^{\circ} =$		-529.12		
	Literatui	re – Calculated:	= Residual	Reference	$\Delta_{r}G^{\circ} =$		234.04		
					$lnK_f =$		- 94.41 		
Gas phase Δ _t H° =	96.65	96.91	-0.26	69STU/WES	Liquid phas				
$C_p^{\circ} =$	184.18	185.14	-0.20	69STU/WES	$\Delta_t H^\circ =$	SC .	9.79		
$S^{\circ} =$	418.15	420.34	- 0.30 - 2.19	69STU/WES	$C_p^{\circ} =$		277.70		
$\Delta_{f}S^{\circ} =$	410.13	-431.97	- 2.19	0931 O/ WE3	$S^{\circ} =$		334.59		
$\Delta_i G^\circ =$		225.70			$\Delta_{f}S^{\circ} =$		-654.03		
$\ln K_0 =$		-91.05			$\Delta_{\rm f}G^{\circ} =$		204.79		
			<u></u>		$\ln K_{\rm f} =$		- 82.61		
iquid phase	e								
$\Delta_t H^\circ =$		35.52		•	2-Propylna		- C /H) /C) \	/1 × 6 /1*	C ₁₃ F
$C_p^{\circ} =$		247.28					\times C-(H) ₂ (C) ₂) +		(C)(C _B))+
S° =		302.21					$2 \times C_{BF}$ (C_{BF})		
$\Delta_f S^\circ = \Delta_f G^\circ =$		-550.10 199.53			(2 × napn	maiche I St	$(1b) + (7 \times C_B - (1$	$1/(CB/2)$, $\sigma =$. 3
$\ln K_{\rm f} =$		- 80.49				Literature	e – Calculated =	= Residual	Reference
	······································				<u> </u>				
2-Ethylnaph		VE 611 1011	· >> - (1 · · · · ·	$C_{12}H_{12}$	Gas phase $\Delta_l H^{\circ}$ –	73.85	76.28	2.43	69STU/WES
		× C-(H) ₂ (C)(C		(C)(C _B) ₂)+	$C_p^{\circ} =$	208.36	208.03	0.33	
) + (2×naphtha	nene i sub)+		$S^{\circ} =$	460.99	459.50	1.49	69STU/WES 69STU/WES
$(7 \times C_B - (1 + C_B))$	1)(CB)2), C	r = 3			$\Delta_{f}S^{\circ} =$	100.77	-529.12	1.77	0/31 U/ WES
	Literatus	re – Calculated	= Residual	Reference	$\Delta_i G^\circ =$		234.04		
	Literatu		- Residual	Reference	$\ln K_{\rm f} =$		-94.41		
Gas phase		•			T:::				
	95.90	96.91	-1.01	69STU/WES	Liquid phas	ie	0.70		
$\Delta_{f}H^{\circ} =$	184.43	185.14	-0.71	69STU/WES	$\Delta_t H^\circ =$		9.79		
$\Delta_t H^\circ = C_p^\circ =$		100.01	0.40	69STU/WES	$C_p^{\circ} =$		277.70		
$C_p^{\circ} = S^{\circ} =$	420.74	420.34	0.40	0931 O/WE3	oʻ-		204 20		
$C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} =$		420.34 -431.97	0.40	0931 U/WE3	S° =		334.59		
S° =			0.40	0931 U/WE3	$S^{\circ} = \Delta_{f}S^{\circ} - \Delta_{f}G^{\circ} =$		334.59 -654.03 204.79		

$(1 \times C_B - (0))$	$(1)_3(C) + (2)^2$ $(2)(C_B)_2 + (3)^2$	$\times C-(H)_2(C)_2)$ $2 \times C_{BF}-(C_{BF})_1$ $1b) + (7 \times C_B-(C_{BF})_1$	$(C_B)_2) +$		1-Pentyinaphthalene (Continued) $(1 \times C - (H)_3(C)) + (3 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)(C_B)) + (1 \times C_B - (C)(C_B)_2) + (2 \times C_{BF} - (C_{BF})(C_B)_2) + (2 \times naphthalene 1 sub) + (7 \times C_B - (H)(C_B)_2), \ \sigma = 3$				
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	53.05 230.87 497.18	55.65 230.92 498.66 -626.27 242.37 -97.77	-2.60 -0.05 -1.48	69STU/WES 69STU/WES 69STU/WES	Liquid pha: $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	se	-41.67 338.54 399.35 -861.89 215.30 -86.85		
Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	se ·	- 15.94 308.12 366.97 - 757.96 210.05 - 84.73			$(1 \times C_{B} \sim ($	$(C)(C_B)_2 + (3)_3$ $(C)(C_B)_2 + (3)_3$ $(C)(C_B)_2 + (3)_3$	\times C-(H) ₂ (C) ₂) (2 \times C _{BF} -(C _{BF})(ub) + (7 \times C _B -(re – Calculated	$(C_B)_2) + H(C_B)_2), \sigma =$	
(1×C _B -($(C)(C_B)_2 + (C)(C_B)_2 + (C)(C_B)_2 + (C)$	× C-(H) ₂ (C) ₂) (2 × C _{BF} -(C _{BF}) (ub) + (7 × C _B -(e – Calculated	$(C_B)_2$) + H)(C_B) ₂), $\sigma =$. ,	Gas phase $ \Delta_t H^\circ = C_p^\circ = C_p^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_f = $	31.67 254.01 539.28	35.02 253.81 537.82 -723.42 250.71 -101.13	-3.35 0.20 1.46	69STU/WES 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t =$	52.30 231.12 499.82	55.65 230.92 498.66 - 626.27 242.37 - 97.77	- 3.35 0.20 1.16	69STU/WES 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^o = C_p^o = S^o = \Delta_t S^o = \ln K_t = $	se	-41.67 338.54 399.35 -861.89 215.30 -86.85		
Liquid phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se	-15.94 308.12 366.97 -757.96 210.05 -84.73		· · · · · · · · · · · · · · · · · · ·	1,2-Dimethy (2×C-(F (2×naph	(C) + (2 thalene 2 s	ne $\times C_{B^{-}}(C)(C_{B})_{2}$ $ub) + (6 \times C_{B^{-}}(I)$ $e - Calculated$	$H)(C_B)_2), \sigma =$: 9
$(1 \times C_B - ($	$(1)_3(C) + (3)_3(C)(C_B)_2 + (3)_3(C)$	× C-(H) ₂ (C) ₂) (2 × C _{BF} -(C _{BF})(ub) + (7 × C _B -(e – Calculated	$(C_B)_2$) + H)($C_B)_2$), $\sigma =$		Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	83.55 184.85 406.81	85.82 185.58 409.01 -443.29 217.99 -87.94	-2.27 -0.73 -2.20	69STU/WES 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	32.43 253.76 536.64	35.02 253.81 537.82 -723.42 250.71 -101.13	-2.59 -0.05 -1.18	69STU/WES 69STU/WES 69STU/WES	Liquid phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_f =$	e	23.72 248.28 289.74 - 562.57 191.45 - 77.23		

		te $(C_B-(C)(C_B)_2)$ $(C_B-(C)(C_B)_2)$			(2×C-(H	(C) + (2	ne (Continued) $\times C_B - (C)(C_B)_2$ $ub) + (6 \times C_B - (C)$	$+(2\times C_{BF}-(0))$	
	Literature	- Calculated :	= Residual	Reference		Literatur	e – Calculated —	= Residual	Reference
Gas phase					Liquid phas	e			
$\Delta_{\mathbf{f}}H^{\circ} =$	81.80	85.82	-4.02	69STU/WES	$\Delta_{\rm f}H^{\circ} =$		23.72		
$C_p^{\circ} =$	185.10	185.58	-0.48	69STU/WES	$C_p^{\circ} =$		248.28		
S° =	409.45	409.01	0.44	69STU/WES	S° =		289.74		
$\Delta_f S^{\circ} =$		- 443.29			$\Delta_f S^\circ =$		- 562.57		
$\Delta_{\rm f}G^{\circ} =$		217.99			$\Delta_{\rm f}G^{\circ} =$		191.45		
$lnK_f =$		– 87.94 ––––––	 		$lnK_f =$				
Liquid phas	:e								
$\Delta_{i}H^{\circ} =$		23.72			1,6-Dimethy				C ₁₂ H
$C_p^{\circ} =$		248.28			(2×C-(H	(C) + (2	$\times C_B - (C)(C_B)_2$	$+(2\times C_{BF}-(0))$	$C_{BF})(C_B)_2) +$
<i>S</i> ° =		289.74			(2×naph	thalene 2 s	ub)+(6×C _B −($H)(C_B)_2), \sigma =$	= 9
$\Delta_r S^{\circ} =$		- 562.57				- •			
$\Delta_f G^\circ = \ln K_f =$		191.45 - 77.23			***	Literatur	e – Calculated	= Residual	Reference
					Gas phase				
					$\Delta_{\rm f} H^{\circ} =$	82.51	85.82	-3.31	69STU/WES
1,4-Dimethy	ylnaphthaler	1e		$C_{12}H_{12}$	$C_p^{\circ} =$	185.10	185.58	-0.48	69STU/WES
,		$\times C_{B}$ -(C)(C _B) ₂)	$)+(2\times C_{BF}-(0))$		S° =	409.45	409.01	0.44	69STU/WES
•	,- , ,, ,	$ab) + (6 \times C_{B} - (1)$		/,	$\Delta_{\mathbf{f}}S^{\circ} =$		-443.29		
` .		•	,-		$\Delta_{\mathbf{f}}G^{\circ} =$		217.99		
	Literatur	e – Calculated	= Residual	Reference	$lnK_f =$		-87.94		
Gas phase					Liquid phas	Α			
$\Delta_{i}H^{\circ} =$	82.51	85.82	-3.31	69STU/WES	$\Delta_t H^\circ =$		23.72		
$C_p^{\circ} =$	184.85	185.58	-0.73	69STU/WES	$C_p^{\circ} =$		248.28		
S° =	401.08	403.25	-2.17	69STU/WES	. S° =		289.74		
$\Delta_f S^\circ =$.01.00	-449.06		0,010,1,20	$\Delta_{f}S^{\circ} =$		- 562.57		
$\Delta_{\mathbf{f}}G^{\circ} =$		219.71			$\Delta_t G^\circ =$		191.45		
$lnK_f =$		-88.63			$lnK_{f} =$		-77.23		
Liquid phas									
$\Delta_{\rm f}H^{\circ} =$		23.72			1,7-Dimethy	-			C ₁₂ H
$C_p^{\circ} =$		248.28					$\times C_{B}$ -(C)(C _B) ₂		
		289.74			(∠× napn	maiene Z SI	$ab) + (6 \times C_{B} - (2)$	$\Pi_{J}(C_{BJ2J}, \sigma =$	· y
S° =		-562.57				I itamatu-	e – Calculated	_ Dasidual	Doforces
$\Delta_f S^{\circ} =$		191.45 77.23				Literatur		= Residuai	Reference
					Gas phase				
$\Delta_f S^\circ = \Delta_f G^\circ =$		¥					05.00	-4.02	69STU/WES
$\Delta_f S^\circ = \Delta_f G^\circ = InK_f =$		Hoper			$\Delta_{\mathbf{f}}H^{\circ} =$	81.80	85.82		
$\Delta_t S^\circ = \Delta_t G^\circ = InK_t = InK_t$	yinaphthale			C ₁₂ H ₁₂	$C_p^{\circ} =$	185.10	185.58	-0.48	69STU/WES
$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_f = \frac{1,5\text{-Dimeth}}{2 \times C - (I)}$	$H)_3(C)) + (2)$	$\times C_{B}$ - $(C)(C_{B})_{2}$		$C_{BF})(C_B)_2) +$	$C_p^\circ = S^\circ =$		185.58 409.01		69STU/WES 69STU/WES
$\Delta_{\rm f}S^{\circ} = \Delta_{\rm f}G^{\circ} = {\rm in}K_{\rm f} $	$H)_3(C)) + (2)$			$C_{BF})(C_B)_2) +$	$C_p^\circ = S^\circ = \Delta_t S^\circ = 0$	185.10	185.58 409.01 - 443.29	-0.48	
$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_f = \frac{1,5\text{-Dimeth}}{2 \times C - (I)}$	H) ₃ (C))+(2) hthalene 2 st	$\times C_{B}$ -(C)(C _B) ₂ ub) + (6 \times C _B -($H)(C_B)_2), \sigma =$	$(C_{BF})(C_{B})_{2}$ + = 9	$C_p^\circ = S^\circ =$	185.10	185.58 409.01 - 443.29 217.99	-0.48	
$\Delta_{\rm f}S^{\circ} = \Delta_{\rm f}G^{\circ} = {\rm in}K_{\rm f} $	H) ₃ (C))+(2) hthalene 2 st	$\times C_{B}$ - $(C)(C_{B})_{2}$	$H)(C_B)_2), \sigma =$	$C_{BF})(C_B)_2) +$	$C_p^\circ = S^\circ = \Delta_t S^\circ = 0$	185.10	185.58 409.01 - 443.29	-0.48	
$\Delta_{\rm f}S^{\circ} = \Delta_{\rm f}G^{\circ} = {\rm in}K_{\rm f} $	H) ₃ (C))+(2) hthalene 2 st	$\times C_{B}$ -(C)(C _B) ₂ ub) + (6 \times C _B -($H)(C_B)_2), \sigma =$	$(C_{BF})(C_{B})_{2}$ + = 9	$C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = 0$	185.10 409.45	185.58 409.01 - 443.29 217.99	-0.48	
$\Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = 1$ 1,5-Dimeth $(2 \times C - (1 \times C + C))$	H) ₃ (C))+(2) hthalene 2 st	$\times C_{B}$ -(C)(C _B) ₂ ub) + (6 \times C _B -($H)(C_B)_2), \sigma =$	$(C_{BF})(C_{B})_{2}$ + = 9	$C_{\rho}^{\circ} = S^{\circ} = S_{f}^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = S_{f}^{\circ}$	185.10 409.45	185.58 409.01 - 443.29 217.99	-0.48	
$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 1,5$ -Dimeth (2×C-(I (2×napl	H) ₃ (C)) + (2 hthalene 2 so Literatur	\times C _B -(C)(C _B) ₂ ub) + (6 \times C _B -(re – Calculated	$(H)(C_B)_2$, $\sigma =$ = Residual	C _{BF})(C _B) ₂) + = 9 Reference	$C_{\rho}^{\circ} =$ $S^{\circ} =$ $\Delta_{t}S^{\circ} =$ $\Delta_{t}G^{\circ} =$ $\ln K_{t} =$ Liquid phas $\Delta_{t}H^{\circ} =$	185.10 409.45	185.58 409.01 - 443.29 217.99 - 87.94	-0.48	
$\Delta_f S^\circ = \Delta_f G^\circ = InK_f = $	H) ₃ (C)) + (2) hthalene 2 so Literatur 81.80	\times C _B -(C)(C _B) ₂ \times C _B -(C)(C _B) ₂ \times C _B -(C) \times Calculated 85.82	$(H)(C_B)_2$, $\sigma =$ $= Residual$ -4.02	C _{BF})(C _B) ₂) + = 9 Reference 69STU/WES	$C_{\rho}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = $ Liquid phas	185.10 409.45	185.58 409.01 - 443.29 217.99 - 87.94	-0.48	
$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 1,5$ -Dimeth (2×C-(I (2×napl) Gas phase $\Delta_t H^\circ = C_p^\circ = 1$	H) ₃ (C)) + (2: hthalene 2 su Literatur 81.80 184.85	\times C _B -(C)(C _B) ₂ \times C _B -(C)(C _B) ₂ \times C _B -(C) \times Calculated 85.82 185.58	$(H)(C_B)_2$, $\sigma =$ = Residual -4.02 -0.73	C _{BF})(C _B) ₂) + = 9 Reference 69STU/WES 69STU/WES	$C_{\rho}^{\circ} =$ $S^{\circ} =$ $\Delta_{t}S^{\circ} =$ $\Delta_{t}G^{\circ} =$ $\ln K_{t} =$ Liquid phas $\Delta_{t}H^{\circ} =$ $C_{\rho}^{\circ} =$	185.10 409.45	185.58 409.01 - 443.29 217.99 - 87.94 23.72 248.28	-0.48	
$\Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = InK_{t} = InK_{t} = InK_{t}$ 1,5-Dimeth (2×C-(I) (2×naph Gas phase $\Delta_{t}H^{\circ} = C_{t}^{\circ} = S^{\circ} = InK_{t}G^{\circ} = InK_{t}G^{\circ}$	H) ₃ (C)) + (2: hthalene 2 su Literatur 81.80 184.85	× C _B -(C)(C _B) ₂ ub) + (6 × C _B -(e - Calculated 85.82 185.58 409.01	$(H)(C_B)_2$, $\sigma =$ = Residual -4.02 -0.73	C _{BF})(C _B) ₂) + = 9 Reference 69STU/WES 69STU/WES	$C_{p}^{\circ} =$ $S^{\circ} =$ $\Delta_{s}S^{\circ} =$ $\Delta_{t}G^{\circ} =$ $\ln K_{t} =$ Liquid phas $\Delta_{t}H^{\circ} =$ $C_{p}^{\circ} =$ $S^{\circ} =$	185.10 409.45	185.58 409.01 - 443.29 217.99 - 87.94 23.72 248.28 289.74	-0.48	

 $C_{12}H_{12}$

TABLE 11. Aromatic CH-02 (80) - Continued

TABLE 11. Aromatic CH-02 (80) - Continued

1,8-Dimethylnaphthalene $C_{12}H_{12}$ $(2 \times C - (H)_3(C)) + (2 \times C_B - (C)(C_B)_2) + (2 \times C_{BF} - (C_{BF})(C_B)_2) +$ $(2 \times \text{naphthalene } 2 \text{ sub}) + (6 \times C_B - (H)(C_B)_2)$

	Literatur	e – Calculated	= Residual	Reference	
Gas phase					
$\Delta_i H^{\circ} =$	108.66	85.82	22.84	74MAN	
$C_p^{\circ} =$		185.58			
Liquid pha	se		e.		
$\Delta_{\mathbf{f}}H^{\circ} =$	41.76	23.72	18.04	74MAN	
$C_p^{\circ} =$		248.28			
S° =		289.74			
$\Delta_t S^\circ =$		- 562.57			
$\Delta_f G^\circ =$		191.45			
$lnK_f =$		-77.23		······································	
Solid phase	•				
$\Delta_{\rm f} H^{\circ} =$	26.10	1.70	24.40	74MAN	
$C_p^{\circ} =$	242.80	213.76	29.04	77FIN/MES	
S° =	224.72	226.88	-2.16	77FIN/MES	
$\Delta_f S^\circ =$		- 625.43			
$\Delta_t G^{\circ} =$		188.17			
$lnK_f =$		- 75.91			

2,3-Dimethylnaphthalene $C_{12}H_{12}$ $(2 \times C - (H)_3(C)) + (2 \times C_B - (C)(C_B)_2) + (2 \times C_{BF} - (C_{BF})(C_B)_2) +$ $(2 \times \text{naphthalene } 2 \text{ sub}) + (6 \times C_B - (H)(C_B)_2), \sigma = 18$

	Literatu	rc — Calculated	- Residual	Reference
Gas phase				
$\Delta_i H^{\circ} =$	83.55	85.82	-2.27	69STU/WES
$C_p^{\circ} =$	185.81	185.58	0.23	69STU/WES
$S^{\circ} =$	410.95	403.25	7.70	69STU/WES
Δ ₁ S° =	410.23	- 449.06	7.70	0701 C/ WED
$\Delta_f G^{ } =$		219.71		
$\ln K_{\rm f} =$		-88.63		
			······································	
Liquid pha	se			
$\Delta_t H^\circ =$		23.72		
$C_p^{\circ} =$		248.28		
S° =		289.74		
Δ ₆ S° =		-562.57		
$\Delta_{\rm f}G^{\circ} =$		191.45		
$lnK_f =$		-77.23		
-				
Solid phase	:			
$\Delta_t H^{\circ} =$	-2.34	1.70	-4.04	73GOO2
$C_p^{\circ} =$		213.76		
5° =		226.88		
Δ ₀ S° =		-625.43		
$\Delta_{\rm f}G^{\circ} =$		188.17		
$\ln K_{\rm f} =$		- 75.91		
		12124		

2,6-Dimethylnaphthalene	$C_{12}H_{12}$
$(2 \times C - (H)_3(C)) + (2 \times C_B - (C)(C_B)_2) + (2 \times C_{BF} - (C_{BF})(C_B)_2) +$	
$(2 \times \text{naphthalene 2 sub}) + (6 \times C_B - (H)(C_B)_2), \sigma = 9$	

	Literatur	e – Calculated	lated = Residual Referen		
Gas phase					
$\Delta_f H^\circ =$	82.51	85.82	-3.31	69STU/WES	
$C_p^{\circ} =$	187.07	185.58	1.49	69STU/WES	
S° =	408.69	409.01	-0.32	69STU/WES	
$\Delta_f S^\circ =$		-443.29			
$\Delta_t G^{\circ} =$		217.99			
$lnK_f =$		-87.94			
Liquid pha	se				
$\Delta_t H^\circ =$		23.72			
$C_p^{\circ} =$		248.28			
S° =		289.74			
$\Delta_f S^\circ =$		-562.57			
$\Delta_f G^\circ =$		191.45			
$lnK_f =$		-77.23			
Solid phase	e				
$\Delta_{\rm f} H^{\circ} =$	-5.73	1.70	−7.43	73GOO2	
$C_p^{\circ} =$	203.55	213.76	- 10.21	77FIN/MES	
s° =	227.86	226.88	0.98	77FIN/MES	
$\Delta_f S^\circ =$		-625.43		•	
$\Delta_f G^\circ =$		188.17			
$lnK_f =$		-75.91			

2,7-Dimethylnaphthalene $(2 \times C - (II)_3(C)) + (2 \times C_{B} - (C)(C_B)_2) + (2 \times C_{BF} - (C_{BF})(C_B)_2) +$ $(2 \times \text{naphthalene } 2 \text{ sub}) + (6 \times C_{B} - (H)(C_{B})_{2}), \sigma = 18$

Literature - Calculated = Residual Reference Gas phase $\Delta_t H^\circ =$ 82.51 85.82 -3.3169STU/WES $C_p^{\circ} = S^{\circ} =$ 187.07 185.58 69STU/WES 1.49 408.69 403.25 5.44 69STU/WES $\Delta_f S^\circ =$ -449.06 $\Delta_f G^\circ =$ 219.71 $lnK_f =$ -88.63Liquid phase $\Delta_{\mathbf{f}}H^{\circ} =$ 23.72 $C_{\rho}^{\circ} = S^{\circ} =$ 248.28 289.74 $\Delta_6 S^\circ =$ ~562.57 $\Delta_f G^{\circ} =$ 191.45 $lnK_f =$ -77.23Solid phase $\Delta_f H^\circ =$ -5.441.70 -7.1473GOO2 $C_p^{\circ} = S^{\circ} =$ 204.39 213.76 -9.3777FIN/MES 228.57 226.88 77FIN/MES 1.69 $\Delta_f S^{\circ} =$

-- 625.43

188.17

-75.91

 $\Delta_f G^\circ =$

 $lnK_f =$

TABLE 11. Aromatic CH-02 (80) - Continued

$(2 \times C_{BF} - ($	$(1)_3(C) + (1 \times$	C-(H)2(C)(C +(2×naphtha		$C_{13}H_{14}$ (C)(C _B) ₂) +	$(2 \times C_{BF})$	$(1)_3(C) + (1)_3(C)$	× C-(H) ₂ (C)(C +(2×naphtha		
	Literature	- Calculated	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	65.77 210.46 457.44	64.48 211.19 451.60 -537.02 224.59 -90.60	1.29 - 0.73 5.84	69STU/WES 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ = C_r^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	61.30 211.71 455.18	64.48 211.19 451.60 -537.02 224.59 -90.60	-3.18 0.52 3.58	69STU/WES 69STU/WES 69STU/WES
Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	e	- 1.09 271.18 337.14 - 651.48 193.15 - 77.91			Liquid phas $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	е	-1.09 271.18 337.14 -651.48 193.15 -77.91		
$(2 \times C - (H))$ $(2 \times C_{BF} - (H))$	$(C_{BF})(C_B)_2$ H) $(C_B)_2$, σ	$< C-(H)_2(C)(C)$ + $(2 \times naphtha)$ = 9	lene 2 sub)+		Tetraphenyl	$(C_B)_2$) + (4 ×	C _B -(C _d)(C _B) ₂) e – Calculated :	•	C ₂₆ H ₂₈ I)(C _B) ₂) Reference
Gas phase	Literature	e – Calculated	= Residual	Reference	Gas phase $\Delta_t H^\circ =$		438.64		
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ - \Delta_t G^\circ = \ln K_t =$	61.30 211.71 455.18	64.48 211.19 451.60 - 537.02 224.59 - 90.60	-3.18 0.52 3.58	69STU/WES 69STU/WES 69STU/WES	Liquid phas $\Delta_t H^\circ = C_p^\circ -$	e	301.34 541.56		
Liquid phas $\Delta_t H^\circ =$	se	-1.09	1 (27)		Solid phase $\Delta_l H^o - C_p^o =$	311.50 387.60	311.50 387.60	0.00 0.00	50COO/HOI 31SMI/AND
$C_{\rho}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = InK_{f} = InK_{f}$		271.18 337.14 -651.48 193.15 -77.91			Anthracene (4×C _{BF}		+ (10×C _B -(H) e – Calculated =		C₁₄H₁₀ Reference
Solid phase $ \Delta_t H^\circ = \\ C_p^\circ = \\ S^\circ = \\ \Delta_t S^\circ = $	•	- 20.40 263.14 253.78 - 734.84			Gas phase $\Delta_t H^\circ = C_p^\circ =$	230,96	218.50 136.10	12.46	64KEL/RIC
$\Delta_t G^\circ = \ln K_t = -$		198.69 - 80.15			Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	e 158.57	144.92 264.88 266.54 - 466.67 284.06 - 114.59	13.65	70GOU/GIR

TABLE 11. Aromatic CH-02 (80) - Continued

TABLE 11. Aromatic CH-02 (80) - Continued

Anthracene (l) +(10×C _B −(H	$(C_B)_2$	C ₁₄ H ₁₀	Triphenylene (6×C _{BF} -()+(12×C _B -(H	I)(C _B) ₂)	C ₁₈ H	
(*** 05)** (Literature - Calculated = Residual				Reference	Literature – Calculated = Residual				Reference
Calid ahasa					Gas phase					
Solid phase $\Delta_t H^\circ =$	129.20	121.70	7.50	66COL/PIL	$\Delta_{\mathbf{f}}H^{\circ} =$	269.80	261.72	8.08	58HOY/PEP	
-		210.50	0.00	70GOU/GIR						
$C_p^{\circ} =$	210.50		3.65	70GOU/GIR						
S° =	207.15	203.50	3.03	/0000/GIK	Liquid phase	•				
$\Delta_{f}S^{\circ} =$		-529.71			$\Delta_t H^\circ =$	176.52	166.92	9.60	71WON/WES	
$\Delta_t G^\circ =$		279.63								
$lnK_f =$		- 112.80								
					Solid phase					
	_			СИ	$\Delta_t H^{\circ} =$	151.80	150.36	1.44	78GOO	
Naphthacen			N(C))	$C_{18}H_{12}$	$C_p^{\circ} =$	259.20	276.18	- 16.98	71WON/WES	
(6 × C _{BF} ($C_{BF}(C_B)_2$	$+(12\times C_{B}-(H$)(C _B) ₂)		<i>S</i> ° =	254.68	285.00	-30.32	71WON/WES	
					$\Delta_{f}S^{\circ} =$		601.75		7211021,1120	
	Literatur	e – Calculated	= Residual	Reference	$\Delta_{\mathbf{f}}G^{\circ} =$		329.77			
					$-\ln K_{\rm f} =$		- 133.03			
					-IIIAf =		- 133.03			
Gas phase									· · · · · · · · · · · · · · · · · · ·	
$\Delta_{\mathbf{f}}H^{\circ} =$	283.50	286.32	-2.82	67WAK/INO	Chrysene				C ₁₈ H ₁	
$C_p^{\circ} =$		163.32			•	Cos)(Co)a)	+ (4 × Cps=(C	n)(Cpr)-)+(12	$\times C_B-(H)(C_B)_2$	
					(Z. OBF (e – Calculated		Reference	
Liquid phase $\Delta_t H^* =$	e	192.90								
-		329.28								
$C_p^{\circ} =$					Gas phase					
S° =		313.20			$\Delta_t H^\circ =$	276.30	269.92	6.38	80KRU	
$\Delta_f S^\circ =$		-573.55								
$\Delta_f G^\circ =$		363.90								
$\ln K_{\rm f} =$		- 146.80			Liquid phase	;				
					$\Delta_f H^\circ =$		175.58			
Solid phase										
$\Delta_t H^{\circ} =$	158.78	162.96	-4.18	51MAG/HAR	Solid phase					
$C_p^{\circ} =$	236.56	255.36	- 18.80	80WON/WES	$\Delta_{\rm f}H^{\circ} =$	145.30	154.56	_ 0.26	513.4.4.0.0TA	
S° =	215.39	237.00	-21.61	80WON/WES		173.30		- 9.26	51MAG/HAR	
$\Delta_{f}S^{\circ} =$	22,007	- 649.75	21.01	557. G17 11 LB	$C_p^{\circ} =$		269.24			
$\Delta_{i}G^{\circ} =$		356.68			S° =		269.00			
					$\Delta_f S^\circ =$		-617.75			
$lnK_f =$		- 143.88			$\Delta_f G^{\circ} =$		338.74			
				•	$lnK_f =$		- 136.65			
Phenanthre)+(2×C _{BF} -(C ₂	B)(CBF)2)+(10	$C_{14}H_{10}$ $0 \times C_{B}-(H)(C_{B})_{2})$	Pyrene (2×C _{BF} -(0	C _{BF}) ₃)+(4	$\times C_{BF}$ $(C_{BF})(C_{BF})$	C _B) ₂)+(10×C _F	C ₁₆ H ₁₆ 1-(H)(C _B) ₂)	
	Literatur	e – Calculated	= Residual	Reference			e – Calculated		Reference	
						<u>.,</u>				
					Gas phase					
Gas phase	209.10	210.30	-1.20	59AIH	$\Delta_i H^\circ =$	225.68	225.68	0.00	80SMI/STE	
Gas phase $\Delta_t H^\circ =$					73					
$\Delta_t H^{\circ} =$					Liquid phase	143.13	143.12	0.01	71WON/WES	
$\Delta_t H^{\circ} =$		136.26	-3.60	77FIN/MES	$\Delta_{\rm f}H^{\circ} =$	143.13		0.01	/1 W O1 V W LS	
Liquid phase Δ _t H° =	e	136.26	-3.60	77FIN/MES		143.13		0.01	71W017/WED	
$\Delta_t H^{\circ} =$ Liquid phase $\Delta_t H^{\circ} =$ Solid phase	e 132.66				Solid phase	······································				
$\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$	e 132.66 116.20	117.50	-1.30	66COL/PIL	Solid phase $\Delta_t H^\circ =$	125.48	125.58	-0.10	80SMI/STE	
$\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_\rho^\circ =$	132.66 116.20 220.62	117.50 217.44	-1.30 3.18	66COL/PIL 77FIN/MES	Solid phase $\Delta_t H^\circ =$	······································			80SMI/STE	
$\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$	e 132.66 116.20	117.50	-1.30	66COL/PIL	Solid phase $\Delta_t H^\circ = C_p^\circ =$	125.48 227.65	125.58 226.50	-0.10 1.15	80SMI/STE 71WON/WES	
$\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_\rho^\circ =$	132.66 116.20 220.62	117.50 217.44	-1.30 3.18	66COL/PIL 77FIN/MES	Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	125.48	125.58 226.50 217.50	-0.10	80SMI/STE	
$\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_t^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$	132.66 116.20 220.62	117.50 217.44 219.50 -513.71	-1.30 3.18	66COL/PIL 77FIN/MES	Solid phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = $	125.48 227.65	125.58 226.50 217.50 - 527.20	-0.10 1.15	80SMI/STE 71WON/WES	
$\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_t^\circ =$ $S^\circ =$	132.66 116.20 220.62	117.50 217.44 219.50	-1.30 3.18	66COL/PIL 77FIN/MES	Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	125.48 227.65	125.58 226.50 217.50	-0.10 1.15	80SMI/STE 71WON/WES	

TABLE 11. Aromatic CH-02 (80) - Continued

TABLE 11.	Aromatic	CH-02	(80) —	Continued
TIME II.	2 HOHatie	CITOL	(00)	Continuou

 $C_{20}H_{12}$

67WES/WON 80WON/WES 80WON/WES

 $C_{24}H_{12}$

1,2-Benzanth (4×C _{BF} -(+ (2×C _{BF} -(C	$(C_{BF})_2 + (12)_2$	$C_{18}H_{12}$ $2 \times C_B - (H)(C_B)_2)$			$\times C_{BF}$ (C_B)(C_B)	$(C_{BF})_2$ + $(2 \times C_B)_2$	$C_{20}H$ F-(C _{BF})(C _B) ₂)+
	Literatur	e – Calculated	l = Residual	Reference	(12×CB)	(re – Calculatec	l = Residual	Reference
Gas phase Δ _i H° =	294.14	278.12	16.02	80KRU	Liquid phas $\Delta_t H^\circ =$	e	173.78		
Liquid phase Δ _ε H° =	e 170.83	184.24	-13.41	51MAG/HAR	Solid phase $\Delta_t H^\circ =$	182.67	158.44	24.23	67WES/WON
Solid phase				- JF - '	$C_p^{\circ} = S^{\circ} =$	274.93 264.55	285.24 283.00	- 10.31 - 18.45	80WON/WES
$ \Delta_t H^\circ = \\ C_\rho^\circ = \\ S^\circ = $		158.76 262.30 253.00			$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-615.23 341.87 -137.91		
$\Delta_f S^\circ = \Delta_f G^\circ =$		-633.75 347.71							
$lnK_f =$		-140.26			Coronene (6×C _{BF} -	(C _{BF}) ₃)+(6	5×C _{BF} −(C _{BF})($(C_B)_2 + (12 \times C_B)_2$	C ₂₄ H _B -(H)(C _B) ₂)
Fluoranthen (1×C _{BF} -($1 \times C_{BF} - (C_{BF})($	$(C_B)_2$ + $(4 \times C_B)_2$	$C_{16}H_{10}$ $C_{16}H_{10}$		Literatur	re – Calculated	l = Residual	Reference
(10×C _B -	· / · -/-/	+ (1 × fluoranti re – Calculated	,	Reference	Gas phase $\Delta_t H^\circ =$		307.86		
Gas phase Δ _i H° =	289.00	289.00	0.00	72MOR2	Liquid phase $\Delta_t H^\circ =$	e	187.50		

Reference

	Literatur	rature - Calculated = Residual Reference				
Gas phase Δ _t H° =	289.00	289.00	0.00	72MOR2		
Liquid pha Δ _t H° =	se 205.00	205.00	0.00	71WON/WES		
Solid phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} =$	e 189.00 230.25 230.58	189.00 230.25 230.58	0.00 0.00 0.00	67WES/WON 71WON/WES 71WON/WES		
$ \Delta_{f}S^{\circ} = \\ \Delta_{f}G^{\circ} = \\ \ln K_{f} = $		-514.11 342.28 -138.07				

Perylene C ₂₀	H ₁₂
$(2 \times C_{BF} - (C_{BF})_3) + (4 \times C_{BF} - (C_B)(C_{BF})_2) + (2 \times C_{BF} - (C_{BF})(C_B)_2) + (2 \times C_{BF} - (C_{BF})_3) + (2 \times C_{BF} - (C_{$	
$(12 \times C_{B}-(H)(C_{B})_{2})$	

Gas phase $\Delta_i H^\circ =$	277.10	

Literature - Calculated = Residual

	Literatu	re – Calculated :	- Calculated = Residual Refere			
Gas phase Δ _f H° =		307.86	100 800 800			
Liquid pha $\Delta_t H^\circ =$	se	187.50				
Solid phase	•					
$\Delta_{\rm f}H^{\circ} =$		174.60				
$C_p^{\circ} =$	313.76	303.36	10.40	80WON/WES		
s° =	280.87	279.00	1.87	80WON/WES		
$\Delta_{f}S^{\circ} =$		-642.19				
$\Delta_f G^{\circ} =$		366.07				
$lnK_f =$		- 147.67				

TABLE 12. Cyclic CH-01 (40)

Cyclopropa (3 × C=(1	ine H}_(C)_) + (1	× Cyclopropan	a = rsc), $a = t$	C ₃ H ₆	Cyclohexa (6×C-(1 × Cyclohexane	rsc (unsub))	C_6H
(3×C-(1		e – Calculated		Reference	(0 × C-(re – Calculated	, ,,	Reference
Gas Phase					Gas Phase				
$\Delta_1 H^{\circ} =$	53.26	53.26	0.00	49KNO/ROS	$\Delta_t H^{\circ} =$	- 123.10	- 123.10	0.00	47OSB/GIN
$C_p^{\circ} =$	55.94	55.94	0.00	69STU/WES	$C_p^{\circ} =$	106.27	106.27	0.00	69STU/WES
S° =	237.44	237.44	0.00	69STU/WES	S° =	298.24	298.24	0.00	69STU/WES
$\Delta_f S^\circ =$		- 171.49			$\Delta_{\mathbf{r}}S^{\circ} =$		-519.62		
$\Delta_r G^{\circ} =$		104.39			$\Delta_{\mathbf{r}}G^{\circ} =$		31.83		
$lnK_f =$		- 42.11			$lnK_f =$		- 12.84		
Liquid Pha	ise				Liquid Ph	ase			
$\Delta_t H^\circ =$		34.39			$\Delta_t H^\circ =$	-156.15	- 156.15	0.00	69GOO/SMI
$C_p^{\circ} =$		62.73			$C_p^{\circ} =$	156.31	156.31	0.00	43RUE/HUF
υp					<i>s</i> ° =	204.35	204.35	0.00	43RUE/HUF
					$\Delta_f S^\circ =$		-613.52		
					$\Delta_{\rm f}G^{\circ} =$		26.77		
Cyclobutan	1e			C₄H ₈	$\ln K_{\rm f} =$		-10.80		
		l × Cyclobutane	rsc), $\sigma = 8$						
	Literatur	e – Calculated:	= Residual	Reference	Cyclohepta		1 × Cycloheptan	o === 2	C7H1
Gas Phase					(/^C-(11)2(C)2) + (1 × Cyclonepian	$e (sc), \sigma = 2$	
$\Delta_c H^\circ =$	28.37	28.37	0.00	50COO/KAR		Literatu	re – Calculated :	= Decidual	Reference
$C_p^{\circ} =$	72.22	72.22	0.00	69STU/WES	Gas Phase		re - Calculated	- Kesiduai	Reference
$S^{\circ} =$	265.39	265.39	0.00	69STU/WES	045 7 7450				
Δ ₆ S° =	203.33	- 279.85	0.00	0931 C/ WE3	$\Delta_{\rm f} H^{\circ} =$	-118.07	- 118.07	0.00	56FIN/SCO
$\Delta_i G^\circ =$		111.81			$C_p^{\circ} =$	123.09	123.09	0.00	
Δ ₁ C =		111.01						UAA	69STU/WES
		45 10							COCTATATATA
$\ln K_f =$		-45.10			S° =	342.33	342.33	0.00	69STU/WES
		-45.10			$S^{\circ} = \Delta_{i}S^{\circ} =$		342.33 -611.85		69STU/WES
	- <u>-</u>	-45.10		· · · · · · · · · · · · · · · · · · ·	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = 0$		342.33 -611.85 64.35		69STU/WES
$\ln K_f =$		-45.10			$S^{\circ} = \Delta_{i}S^{\circ} =$		342.33 -611.85		69STU/WES
$lnK_f =$ Cyclopenta			e rsc (unsub)	C_5H_{10} C_5H_{10}	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$	342.33	342.33 -611.85 64.35		69STU/WES
$lnK_f =$ Cyclopenta		-45.10	e rsc (unsub)		$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = $ Liquid Pha	342.33	342.33 - 611.85 64.35 - 25.96	0.00	
$lnK_f =$ Cyclopenta	$H)_2(C)_2) + (1$		` ,		$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{\Delta_{t}H^{\circ}}$ Liquid Pha	342.33 use - 156.61	342.33 -611.85 64.35 -25.96	0.00	52KAA/COO
$lnK_f =$ Cyclopenta	$H)_2(C)_2) + (1$	× Cyclopentan	` ,), $\sigma = 10$	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{\Delta_{t}H^{\circ}} = C_{p}^{\circ} = \frac{1}{\Delta_{t}H^{\circ}}$	342.33 use - 156.61 180.75	342.33 -611.85 64.35 -25.96 -156.61 180.75	0.00 0.00 0.00	52KAA/COO 56FIN/SCO
$lnK_f =$ Cyclopenta	$H)_2(C)_2) + (1$	× Cyclopentan	` ,), $\sigma = 10$	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ} = S^{\circ}}{S^{\circ}} = \frac{1}{\Delta_{t}G^{\circ}}$	342.33 use - 156.61	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55	0.00	52KAA/COO
$lnK_f =$ Cyclopenta	H) ₂ (C) ₂) + (1 Literatur	× Cyclopentan	` ,), $\sigma = 10$	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \frac{\Delta_{t}S^{\circ}}{\Delta_{t}} = \frac{\Delta_{t}S^{\circ} = \Delta_{t}S^{\circ}}{\Delta_{t}S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{\Delta_{t}S^{\circ}} = \frac{\Delta_{t}$	342.33 use - 156.61 180.75	342.33 - 611.85 64.35 - 25.96 - 156.61 180.75 242.55 - 711.63	0.00 0.00 0.00	52KAA/COO 56FIN/SCO
$\frac{\ln K_f}{\text{Cyclopenta}}$ $(5 \times \text{C-(1)})$ Gas Phase $\Delta_t H^{\circ} =$	H) ₂ (C) ₂) + (1 Literatur	× Cyclopentan	` ,), $\sigma = 10$	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{S^{\circ}} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \frac{\Delta_{t}G^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}$	342.33 use - 156.61 180.75	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56	0.00 0.00 0.00	52KAA/COO 56FIN/SCO
$\frac{\ln K_f = \frac{1}{\sqrt{5 \times C - (1)}}}{Cyclopenta}$ $(5 \times C - (1))$ Gas Phase	H) ₂ (C) ₂) + (1 Literatur	l × Cyclopentan re – Calculated =	= Residual), σ = 10 Reference	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \frac{\Delta_{t}S^{\circ}}{\Delta_{t}} = \frac{\Delta_{t}S^{\circ} = \Delta_{t}S^{\circ}}{\Delta_{t}S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{\Delta_{t}S^{\circ}} = \frac{\Delta_{t}$	342.33 use - 156.61 180.75	342.33 - 611.85 64.35 - 25.96 - 156.61 180.75 242.55 - 711.63	0.00 0.00 0.00	52KAA/COO 56FIN/SCO
Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^\circ = C_t^\circ = S^\circ = S^\circ = C_t^\circ$	H) ₂ (C) ₂) + (1 Literatur – 76.40	l × Cyclopentan re – Calculated = – 76.40	= Residual	Reference 59MCC/PEN	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{S^{\circ}} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \frac{\Delta_{t}G^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}$	342.33 use - 156.61 180.75	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56	0.00 0.00 0.00	52KAA/COO 56FIN/SCO
Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^\circ = C_t^\circ = S^\circ = S^\circ = C_t^\circ$	H) ₂ (C) ₂) + (1 Literatur - 76.40 83.01	x Cyclopentan e — Calculated = - 76.40 83.01	= Residual 0.00 0.00	Reference 59MCC/PEN 69STU/WES	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{S^{\circ}} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}G^{\circ}}{\Delta_{t}} = \frac{\Delta_{t}G$	342.33 ase - 156.61 180.75 242.55	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56	0.00 0.00 0.00	52KAA/COO 56FIN/SCO 56FIN/SCO
$\frac{\ln K_f}{\ln (5 \times C - 1)}$ Cyclopenta $(5 \times C - 1)$ Gas Phase $\Delta_t H^{\circ} = C_{\rho}^{\circ} = C_{$	H) ₂ (C) ₂) + (1 Literatur - 76.40 83.01	- 76.40 83.01 292.88	= Residual 0.00 0.00	Reference 59MCC/PEN 69STU/WES	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid Pha $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Cyclooctan	342.33 ase - 156.61 180.75 242.55	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41	0.00 0.00 0.00 0.00	52KAA/COO 56FIN/SCO
Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_{\iota} H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{\iota} S^{\circ} = \Delta_{\iota} S^{\circ} = 0$	H) ₂ (C) ₂) + (1 Literatur - 76.40 83.01	- 76.40 83.01 292.88 - 388.68	= Residual 0.00 0.00	Reference 59MCC/PEN 69STU/WES	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid Pha $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Cyclooctan	342.33 use - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41	0.00 0.00 0.00 0.00	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₁₆
Gas Phase $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = C_t K_t K_t $	H) ₂ (C) ₂) + (1 Literatur - 76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48	= Residual 0.00 0.00	Reference 59MCC/PEN 69STU/WES	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = C^{\circ}_{t} = \frac{S^{\circ}}{\Delta_{t}G^{\circ}} = \ln K_{t} = \frac{\Delta_{t}G^{\circ}}{(8 \times C - (10 \times 10^{\circ})^{\circ})^{\circ}}$	342.33 use - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41	0.00 0.00 0.00 0.00	52KAA/COO 56FIN/SCO 56FIN/SCO
Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^{\circ} = C_t^{\circ} = S^{\circ} = \Delta_t S^{\circ} = L_t G^{\circ} = L_t G^{\circ}$ Liquid Pha	H) ₂ (C) ₂) + (1 Literatur - 76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48 - 15.93	0.00 0.00 0.00 0.00	Reference 59MCC/PEN 69STU/WES 69STU/WES	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}G^{\circ} = \ln K_{t}}{(8 \times C - (1))^{3}}$	342.33 use - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41 	0.00 0.00 0.00 0.00 0.00	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₁₆ Reference
Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = InK_{t} = InK_{t}$ Liquid Pha $\Delta_{t}H^{\circ} = InK_{t} = InK_{t}$	-76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48 - 15.93	0.00 0.00 0.00 0.00	Reference 59MCC/PEN 69STU/WES 69STU/WES	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{r}^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t}}{(8 \times C - (1))}$ Gas Phase $\Delta_{t}H^{\circ} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{t}G^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{t}G^{\circ}}{\Delta_{t}G^{\circ}} = \frac{C_{t}G^$	342.33 use - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1 Literatur - 124.39	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41 A × Cyclooctane re - Calculated =	0.00 0.00 0.00 0.00 rsc), σ = 8 ≈ Residual	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₁₆ Reference
In $K_t =$ Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_t G^{\circ} = InK_t =$ Liquid Pha $\Delta_t H^{\circ} = C_{\rho}^{\circ} = C_{\rho}^{\circ}$	-76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48 - 15.93	0.00 0.00 0.00 0.00	Reference 59MCC/PEN 69STU/WES 69STU/WES 46JOH/PRO 46DOU/HUF2	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t}} = \frac{\Delta_{t}G^{\circ} = \ln K_{t}}{(8 \times C - (1))}$ Gas Phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = C_{p}^{\circ$	342.33 use - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1 Literatur - 124.39 139.95	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41 A × Cyclooctane re - Calculated =	0.00 0.00 0.00 0.00 0.00 rsc), σ = 8 ≈ Residual	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₁₆ Reference 56FIN/SCO 69STU/WES
In $K_t =$ Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = InK_t =$ Liquid Pha $\Delta_t H^\circ = C_\rho^\circ = S^\circ = S$	-76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48 - 15.93	0.00 0.00 0.00 0.00	Reference 59MCC/PEN 69STU/WES 69STU/WES	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t}}{(8 \times C - (1))}$ Gas Phase $\Delta_{t}H^{\circ} = \frac{C_{t}H^{\circ}}{C_{t}H^{\circ}} = \frac{C_{t}H^{\circ}}{C_{t}H^{\circ}} = \frac{C_{t}H^{\circ}}{S^{\circ}} = \frac{C_{t}H^{\circ}}{$	342.33 use - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1 Literatur - 124.39	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41 A × Cyclooctane re - Calculated = -124.39 139.95 366.77	0.00 0.00 0.00 0.00 rsc), σ = 8 ≈ Residual	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₁₆ Reference
In $K_f =$ Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_f =$ Liquid Pha $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S$	-76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48 - 15.93	0.00 0.00 0.00 0.00	Reference 59MCC/PEN 69STU/WES 69STU/WES 46JOH/PRO 46DOU/HUF2	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}G^{\circ} = L_{t}G^{\circ}}{(8 \times C - (1))}$ Gas Phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \frac{\Delta_{t}S^{\circ}}{\Delta_{t}S^{\circ}} = \frac{\Delta_{t}S^{\circ}$	342.33 use - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1 Literatur - 124.39 139.95	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41 A × Cyclooctane re - Calculated = -124.39 139.95 366.77 -723.72	0.00 0.00 0.00 0.00 0.00 rsc), σ = 8 ≈ Residual	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₁₆ Reference 56FIN/SCO 69STU/WES
In $K_f =$ Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_f =$ Liquid Pha $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S$	-76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48 - 15.93 - 105.81 128.78 204.14 - 477.41 36.53	0.00 0.00 0.00 0.00	Reference 59MCC/PEN 69STU/WES 69STU/WES 46JOH/PRO 46DOU/HUF2	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\ln K_{t}} = \frac{\Delta_{t}G^{\circ}}{(8 \times C - (1))}$ Gas Phase $\Delta_{t}H^{\circ} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}S^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}$	342.33 use - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1 Literatur - 124.39 139.95	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41 A × Cyclooctane re - Calculated = -124.39 139.95 366.77 -723.72 91.39	0.00 0.00 0.00 0.00 0.00 rsc), σ = 8 ≈ Residual	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₁₆ Reference 56FIN/SCO 69STU/WES
In $K_f =$ Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_f =$ Liquid Pha $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S$	-76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48 - 15.93	0.00 0.00 0.00 0.00	Reference 59MCC/PEN 69STU/WES 69STU/WES 46JOH/PRO 46DOU/HUF2	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}G^{\circ} = L_{t}G^{\circ}}{(8 \times C - (1))}$ Gas Phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \frac{\Delta_{t}S^{\circ}}{\Delta_{t}S^{\circ}} = \frac{\Delta_{t}S^{\circ}$	342.33 use - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1 Literatur - 124.39 139.95	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41 A × Cyclooctane re - Calculated = -124.39 139.95 366.77 -723.72	0.00 0.00 0.00 0.00 0.00 rsc), σ = 8 ≈ Residual	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₁₆ Reference 56FIN/SCO 69STU/WES
In $K_f =$ Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = InK_f =$ Liquid Pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S$	-76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48 - 15.93 - 105.81 128.78 204.14 - 477.41 36.53	0.00 0.00 0.00 0.00	Reference 59MCC/PEN 69STU/WES 69STU/WES 46JOH/PRO 46DOU/HUF2	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\ln K_{t}} = \frac{\Delta_{t}G^{\circ}}{(8 \times C - (1))}$ Gas Phase $\Delta_{t}H^{\circ} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\ln K_{t}} = \frac{\Delta_{t}G^{\circ}}{\ln K_{t$	342.33 ase - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1 Literatur - 124.39 139.95 366.77	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41 A × Cyclooctane re - Calculated = -124.39 139.95 366.77 -723.72 91.39 -36.86	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₁₆ Reference 56FIN/SCO 69STU/WES
In $K_f =$ Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = InK_f =$ Liquid Pha $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S$	-76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48 - 15.93 - 105.81 128.78 204.14 - 477.41 36.53	0.00 0.00 0.00 0.00	Reference 59MCC/PEN 69STU/WES 69STU/WES 46JOH/PRO 46DOU/HUF2	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\ln K_{t}} = \frac{Cyclooctan}{(8 \times C - (1))}$ Gas Phase $\Delta_{t}H^{\circ} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}S^{\circ}}{\ln K_{t}} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{t}G^{\circ}}{\Delta_{t}H^{\circ}} = C_$	342.33 ase - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1 Literatur - 124.39 139.95 366.77	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41 1 × Cyclooctane re - Calculated = -124.39 139.95 366.77 -723.72 91.39 -36.86	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₃₀ Reference 56FIN/SCO 69STU/WES
In $K_f =$ Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = InK_f =$ Liquid Pha $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S$	-76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48 - 15.93 - 105.81 128.78 204.14 - 477.41 36.53	0.00 0.00 0.00 0.00	Reference 59MCC/PEN 69STU/WES 69STU/WES 46JOH/PRO 46DOU/HUF2	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\ln K_{t}} = \frac{Cyclooctan}{(8 \times C - (1))}$ Gas Phase $\Delta_{t}H^{\circ} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\ln K_{t}} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{C_{p}^{\circ}} = \frac{C_{p}^{\circ}}{\Delta_{t}H^{\circ}} $	342.33 ase - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1 Literatur - 124.39 139.95 366.77	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41 A × Cyclooctane re - Calculated = -124.39 139.95 366.77 -723.72 91.39 -36.86	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₁₀ Reference 56FIN/SCO 69STU/WES 69STU/WES
In $K_f =$ Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = InK_f =$ Liquid Pha $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S$	-76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48 - 15.93 - 105.81 128.78 204.14 - 477.41 36.53	0.00 0.00 0.00 0.00	Reference 59MCC/PEN 69STU/WES 69STU/WES 46JOH/PRO 46DOU/HUF2	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\ln K_{t}} = \frac{Cyclooctan}{(8 \times C - (1))^{2}}$ Gas Phase $\Delta_{t}H^{\circ} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}S^{\circ}}{\ln K_{t}} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{S^{\circ}}{S^{\circ}} = S$	342.33 ase - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1 Literatur - 124.39 139.95 366.77	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41 1 × Cyclooctane re - Calculated = -124.39 139.95 366.77 -723.72 91.39 -36.86	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₁₀ Reference 56FIN/SCO 69STU/WES 69STU/WES
In $K_f =$ Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = InK_f =$ Liquid Pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S$	-76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48 - 15.93 - 105.81 128.78 204.14 - 477.41 36.53	0.00 0.00 0.00 0.00	Reference 59MCC/PEN 69STU/WES 69STU/WES 46JOH/PRO 46DOU/HUF2	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\ln K_{t}} = \frac{C_{y} \cos \Delta_{t}G^{\circ}}{(8 \times C - (1))} = \frac{C_{y} \cos \Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\ln K_{t}} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\Delta_{t}S^{\circ}} = \frac{C_{p}^{\circ}}{\Delta_{t}S^{\circ}} = \frac{C_{p}^{\circ}}{\Delta_{t}$	342.33 ase - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1 Literatur - 124.39 139.95 366.77	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41 A × Cyclooctane re - Calculated = -124.39 139.95 366.77 -723.72 91.39 -36.86	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₁₆ Reference 56FIN/SCO 69STU/WES 69STU/WES
In $K_f =$ Cyclopenta $(5 \times C - (1))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = InK_f =$ Liquid Pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S$	-76.40 83.01 292.88	- 76.40 83.01 292.88 - 388.68 39.48 - 15.93 - 105.81 128.78 204.14 - 477.41 36.53	0.00 0.00 0.00 0.00	Reference 59MCC/PEN 69STU/WES 69STU/WES 46JOH/PRO 46DOU/HUF2	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}G^{\circ}}{\ln K_{t}} = \frac{Cyclooctan}{(8 \times C - (1))^{2}}$ Gas Phase $\Delta_{t}H^{\circ} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}S^{\circ}}{\ln K_{t}} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = \frac{C_{p}^{\circ}}{S^{\circ}} = \frac{S^{\circ}}{S^{\circ}} = S$	342.33 ase - 156.61 180.75 242.55 e H) ₂ (C) ₂) + (1 Literatur - 124.39 139.95 366.77	342.33 -611.85 64.35 -25.96 -156.61 180.75 242.55 -711.63 55.56 -22.41 1 × Cyclooctane -124.39 139.95 366.77 -723.72 91.39 -36.86 -167.74 215.48 262.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	52KAA/COO 56FIN/SCO 56FIN/SCO C ₈ H ₁₆ Reference 56FIN/SCO 69STU/WES 69STU/WES

TABLE 12. Cyclic CH-01 (40) - Continued

Cyclononan (9×C-(F		l × Cyclononane	rsc)	C ₉ H ₁₈	Cyclotridecane (Continued) $(13 \times C - (H)_2(C)_2) + (1 \times Cyclotridecane rsc)$	C ₁₃ H ₂
				Reference	Literature – Calculated = Residual	Reference
Gas Phase Δ _t H° =	-132.76	- 132.76	0.00	57KAM	Liquid Phase $\Delta_t H^{\circ} = -309.66 -309.66$ 0.00	60COO/KAM
Liquid Phas Δ _ε H° =		- 181.17	0.00	52KAA/COO	Cyclotetradecane $(14 \times C - (H)_2(C)_2) + (1 \times Cyclotetradecane rsc)$	C ₁₄ H ₂
Cyclodecan		/1 × C1- 1		C ₁₀ H ₂₀	Literature – Calculated = Residual	Reference
(10×C-(. , , , , , , , , , , , , , , , , , , ,	(1 × Cyclodecane re – Calculated =	•	Reference	Gas Phase $\Delta_t H^\circ = -239.45 -239.45$ 0.00	57KAM
Gas Phase $\Delta_t H^\circ =$	-154.31	- 154.31	0.00	57KAM	Solid Phase $\Delta_t H^\circ = -374.26 -374.26$ 0.00	60COO/KAM
Liquid Pha Δ _t H° =		206.69	0.00	60COO/KAM	Cyclopentadecane $(15 \times C - (H)_2(C)_2) + (1 \times Cyclopentadecane rsc)$	C ₁₅ H ₃
Cyclounded		(1×Cycloundec	ane rsc)	C ₁₁ H ₂₂	Literature – Calculated ≈ Residual	Reference
	`	re – Calculated =	,	Reference	Gas Phase $\Delta_t H^\circ = -301.42 -301.42$ 0.00	57KAM
Gas Phase $\Delta_t H^\circ =$	-179.37	-179.37	0.00	57KAM	Solid Phase $\Delta_t H^\circ = -376.06 -376.06 0.00$	60COO/KAM
Liquid Pha $\Delta_t H^\circ =$		- 235.48	0.00	60COO/KAM	Cyclohexadecane $(16 \times C - (H)_2(C)_2) + (1 \times Cyclohexadecane rsc)$	C ₁₆ H ₃ ;
Cyclododec (12 × C-		(1×Cyclododec	ane rsc)	C ₁₂ H ₂₄	Literature – Calculated = Residual	Reference
	Literatu	re – Calculated =	= Residual	Reference	Gas Phase $\Delta_t H^\circ = -321.67 - 321.67 0.00$	57KAM
Gas Phase $\Delta_t H^\circ =$	-230.25	-230.25	0.00	57KAM	Solid Phase $\Delta_t H^{\circ} = -403.42 -403.42 0.00$	60COO/KAM
Solid Phase $\Delta_t H^\circ =$		-306.65	0.00	60COO/KAM	Cycloheptadecane $(17 \times C - (H)_2(C)_2) + (1 \times Cycloheptadecane rsc)$	C ₁₇ H ₃ ,
Cyclotrideo (13×C-		(1×Cyclotrideca	ane rsc)	C ₁₃ H ₂₆	Literature – Calculated = Residual	Reference
		re – Calculated =	•	Reference	Gas Phase $\Delta_t H^\circ = -364.30 -364.30$ 0.00	57KAM
Gas Phase Δ _f H° =	-246.35	-246.35	0.00	57KAM	Solid Phase $\Delta_t H^\circ = -430.41 -430.41 0.00$	60COO/KAM

TABLE 12.	Cyclic CH-	01 (40)	_	Continued
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Cycloproper (2×C _d -(1		< C−(H) ₂ (C _d) ₂)	+ (1 × Cyclop	C ₃ H ₄ oropene rsc)			$\times C - (H)_2(C)(C)$	C _d))+(2×C _d -	C ₆ H ₁₀ -(H)(C))+
	Literature	e – Calculated =	Residual	Reference	(2 6)0	•	e – Calculated =	= Residual	Reference
		276.98 × C-(H) ₂ (C)(C ₀ , $\sigma = 2$	0.00	62WIL/BAR C4H6	Liquid Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	- 38.20 148.36 214.60	-38.78 148.36 214.60 -472.69 102.15 -41.21	0.58 0.00 0.00	69GOO/SMI 77HAI/SUG2 77HAI/SUG2
Gas Phase	Literatur	e – Calculated =	= Residual	Reference			:×C-(H)₂(C)(C	^l d))+(2×Cd-	C ₇ H ₁₂ -(H)(C))+
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	156.69 67.07 263.51	156.69 67.07 263.51 - 151.17	0.00 0.00 0.00	68WIB/FEN 69STU/WES 69STU/WES		•	e – Calculated =	= Residual	Reference
$\Delta_f G^\circ = \ln K_f =$		201.76 -81.39			Gas Phase $\Delta_t H^\circ =$	- 9.20	-9.20	0.00	39CON/KIS
	H) ₂ (C) ₂)+(2 opentene rs	$C \times C_d$ —(H)(C)) + C (unsub)), $\sigma =$ C =	= 2	C_5H_8 $(C)(C_d)) +$ Reference		$I)_2(C)_2) + (2)$ soctene rsc)	:× C-(H)2(C)(C e – Calculated =		C ₈ H ₁₄ -(H)(C))+ Reference
Gas Phase $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} =$	34.43 75.10 289.66	34.43 75.10 289.66	0.00 0.00 0.00	50FOR/CAM 69STU/WES 69STU/WES	Gas Phase Δ _t H° =	- 26.99	- 26.99	0.00	39CON/KIS
$\Delta_f S^\circ = \Delta_f G^\circ - \ln K_f =$		-261.33 112.34 -45.32			Liquid Phas Δ _t H° –	e – 74.02	-74.02	0.00	71ROG/MCL
Liquid Pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$	6.36 122.38 201.25	6.36 122.38 201.25 - 349.73	0.00 0.00 0.00	37DOL/GRE 48HUF/EAT 48HUF/EAT		H)(C)) (1 yclopentadi	× C-(H) _z (C _d) _z) ene rsc) e – Calculated =		C_sH_{ϵ} $(C_d)) +$ Reference
$\Delta_f G^\circ = InK_f =$		110.63 - 44.63			Gas Phase $\Delta_t H^\circ =$	134.35	134.35	0.00	36KIS/RUE2
		$2 \times C - (H)_2(C)(C)$ $\sigma = 2$	C _d)) + (2 × C _d -	C_6H_{10} -(H)(C))+	Liquid Phas $\Delta_t H^\circ =$	e 105.98	105.98	0.00	65HUL/REI
	Literatur	e – Calculated =	= Residual	Reference		$()_2(C)(C_d))$	+ (2 × C₀–(H)(C))+(2×C _d -($C_{\varepsilon}H_{s}$ $(H)(C_{d}))+$
Gas Phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$	- 4.73 105.02 310.75	-4.77 105.02 310.75	0.04 0.00 0.00	50FOR/CAM 69STU/WES 69STU/WES	(1 × 1,3-C	yclohexadie Literature	ne rsc) e – Calculated =	Residual	Reference
$\Delta_f S^* = \Delta_f G^* = \ln K_f =$		-376.55 107.50 -43.36			Gas Phase $\Delta_t H^\circ =$	104.58	104.58	0.00	89STE/CHI

TABLE 12. Cyclic CH-01 (40) - Continued

Liquid Phase $\Delta_H H^2 = 71.41 71.41 0.00 89STE/CHI \Delta_H H^2 = 183.68 183.68 0.00 3000 30000 300000 300000 3000000 30000000 30000000 300000000$	Reference 39CON/KIS 69STU/WES 69STU/WES
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	69STU/WES
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	69STU/WES
$S^{\circ} = 197.28 197.28 0.00 76GEI/WOL \qquad S^{\circ} = 315.64 315.64 0.00 64.56$ $\Delta_{A}S^{\circ} = -359.44 \qquad \Delta_{A}S^{\circ} = -246.83$ $\Delta_{A}G^{\circ} = 178.58 \qquad \Delta_{A}G^{\circ} = 257.27 1nK_{I} = -103.78$ $1,3-Cycloheptadiene \qquad C_{I} = 10.0000000000000000000000000000000000$	•
$ \Delta_{A}S^{\circ} = -359.44 \qquad \Delta_{A}S^{\circ} = -246.83 \\ \Delta_{A}G^{\circ} = 178.58 \qquad \Delta_{A}G^{\circ} = 257.27 \\ \ln K_{I} = -72.04 \qquad \ln K_{I} = -103.78 $ Liquid Phase $ (1 \times C - (H)_{2}(C)_{2}) + (2 \times C - (H)_{2}(C)_{3}) + (2 \times C_{I} - (H)(C)) + 4 \\ (2 \times C_{I} - (H)(C_{3})) + (1 \times 1,3 - C)_{2} + C)_{2} + C + C \\ (1 \times C - (H)_{2}(C)_{3}) + (2 \times C_{I} - (H)(C)) + 4 \\ (2 \times C_{I} - (H)(C_{3})) + (1 \times 1,3 - C)_{2} + C)_{3} + C \\ (2 \times C_{I} - (H)(C_{3})) + (1 \times 1,3 - C)_{2} + C)_{3} + C \\ (2 \times C_{I} - (H)(C_{3})) + (1 \times 1,3 - C)_{2} + C)_{3} + C \\ (3 \times C_{I} - (H)(C_{3})) + (1 \times 1,3 - C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{2} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C \\ (4 \times C_{I} - (H)(C_{3})) + (1 \times C)_{3} + C \\ (4$	69STU/WES
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
I,3-Cycloheptadiene C,H ₁₀ C C,C C C C C C C C C C C C C C C C	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56FIN/SCO
Literature − Calculated = Residual Reference $A_tS^\circ = 214.64 214.64 0.00 50 0.06$ $A_tG^\circ = 248.68 0.06$ $A_tG^\circ = -100.32$ $A_tG^\circ = -10$	56FIN/SCO
Literature – Calculated = Residual Reference $A_tG^\circ = -347.82$ $A_tG^\circ = 248.68$ $InK_t = -100.32$ Gas Phase $A_tH^\circ = 94.35$ 94.35 0.00 39CON/KIS Cyclooctatetraene $(8 \times C_{\sigma} - (H)(C_{\sigma})) + (1 \times Cyclooctatetraene rsc), \sigma = 4$ Literature – Calculated = Residual Reference $(8 \times C_{\sigma} - (H)(C_{\sigma})) + (1 \times Cyclooctatetraene rsc)$ Literature – Calculated = Residual Reference $A_tH^\circ = 297.61$ 297.61 0.00 4 $C_p^\circ = 122.01$ 122.01 0.00 6 Gas Phase $C_p^\circ = 122.01$ 122.01 0.00 6 $C_p^\circ = 122.01$ 122.01 122.01 0.00 6	56FIN/SCO
$ \Delta_t G^\circ = 248.68 \\ \ln K_t = -100.32 $ Gas Phase $ \Delta_t H^\circ = 94.35 94.35 94.35 0.00 39\text{CON/KIS} $ $ Cyclooctatetraene \\ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctatetraene \text{ rsc}), \sigma = 4 $ $ (8 \times C_{\sigma^-}(H)(C_0)) + (1 \times Cyclooctate$	
Gas Phase $\Delta_t H^\circ = 94.35$ 94.35 9.00 39CON/KIS Cyclooctatetraene (8×C _σ -(H)(C _σ)) + (1×Cyclooctatetraene rsc), $\sigma = 4$ 1,4-Cyclohexadiene (4×C _σ -(H)(C)) + (2×C-(H) ₂ (C _σ) ₂) + (1×1,4-Cyclohexadiene rsc) Literature – Calculated = Residual Reference Gas Phase $\Delta_t H^\circ = 297.61 $	
$ \Delta_{e}H^{\circ} = 94.35 94.35 0.00 39\text{CON/KIS} $ $ (8 \times C_{\sigma} - (H)(C_{d})) + (1 \times Cyclooctatetraene \text{ rsc}), \ \sigma = 4 $ $ (4 \times C_{\sigma} - (H)(C)) + (2 \times C - (H)_{2}(C_{d})_{2}) + (1 \times 1, 4 - Cyclohexadiene \text{ rsc}) $ $ Literature - Calculated = Residual Reference $ $ Gas \text{ Phase} $ $ C_{\rho}^{\circ} = 122.01 122.01 0.00 400 $ $ C_{\rho}^{\circ} = 122.01 122.01 0.00 600 $ $ C_{\rho}^{\circ} = 122.01 0.00 600 $	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	СП
1,4-Cyclohexadiene (4 × C _o -(H)(C)) + (2 × C-(H) ₂ (C _o) ₂) + (1 × 1,4-Cyclohexadiene rsc) Literature – Calculated = Residual Reference Gas Phase $\Delta_t H^\circ = 297.61$ 297.61 0.00 4 C° = 122.01 122.01 0.00 6 $\Delta_t H^\circ = 104.75$ 104.75 0.00 89STE/CHI $\Delta_t G^\circ = 326.77$ 326.77 0.00 6 $\Delta_t H^\circ = 104.75$ 104.75 0.00 89STE/CHI $\Delta_t G^\circ = 369.59$ 10.00 6 Liquid Phase $\Delta_t H^\circ = 69.70$ 69.70 0.00 89STE/CHI $C_\rho^\circ = 145.94$ 145.94 0.00 76GEI/WOL Liquid Phase $S^\circ = 189.37$ 189.37 0.00 76GEI/WOL $\Delta_t H^\circ = 254.51$ 254.51 0.00 5 $\Delta_t G^\circ = 179.23$ 5° 220.29 20.29 0.00 4 $\Delta_t G^\circ = 179.23$ 5° 220.29 20.29 0.00 4 $\Delta_t G^\circ = 358.24$ 10.00 - 10.00	C ₈ H
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	•
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Reference
Gas Phase $ \Delta_t H^\circ = 104.75 104.75 0.00 89STE/CHI \qquad \Delta_t S^\circ = 326.77 326.77 0.00 60 0.00 60 0.00 60 0.00 60 0.00 60 0.00 60 0.0$	
Gas Phase $S^{\circ} = 326.77 326.77 0.00 6000 80000 800000 800000 800000 800000 800000 800000 800000 8000000 8000000 8000000 8000000 8000000 8000000 800000000$	49SCO/GRO
$ \Delta_t H^\circ = \ 104.75 104.75 0.00 89STE/CHI \qquad \Delta_t S^\circ = -241.43 \\ \Delta_t G^\circ = 369.59 \\ \ln K_t = -149.09 $ Liquid Phase $ \Delta_t H^\circ = 69.70 69.70 0.00 89STE/CHI \\ C^\circ_p = 145.94 145.94 0.00 76GEI/WOL Liquid Phase \\ S^\circ = 189.37 189.37 0.00 76GEI/WOL \Delta_t H^\circ = 254.51 254.51 0.00 5 \\ \Delta_t S^\circ = -367.35 C^\circ_p = 185.18 185.18 0.00 4 \\ \Delta_t G^\circ = 179.23 S^\circ = 220.29 220.29 0.00 4 \\ \Delta_t S^\circ = -347.91 \Delta_t S^\circ = -347.91 \\ \Delta_t G^\circ = 358.24 10K_t = -144.51 $ $ 1,5-Cyclooctadiene \\ (4 \times C_\sigma - (H)(C)) + (4 \times C - (H)_2(C)(C_d)) + \\ (1 \times 1,5-Cyclooctadiene rsc) $ Spiropentane $ (4 \times C - (H)_2(C)_2) + (1 \times C - (C)_4) + (1 \times Spiropentane rsc) $	59STU/WES
Liquid Phase $\Delta_t G^\circ = 369.59$ $\ln K_t = -149.09$ Liquid Phase $\Delta_t H^\circ = 69.70 69.70 0.00 89STE/CHI$ $C_p^\circ = 145.94 145.94 0.00 76GEI/WOL$ $S^\circ = 189.37 189.37 0.00 76GEI/WOL$ $\Delta_t S^\circ = -367.35 C_p^\circ = 185.18 185.18 0.00 4$ $\Delta_t G^\circ = 179.23 S^\circ = 220.29 220.29 0.00 4$ $\Delta_t S^\circ = -72.30 \Delta_t S^\circ = -347.91 \Delta_t S^\circ = 358.24$ $\ln K_t = -144.51$ 1,5-Cyclooctadiene $(4 \times C_\sigma - (H)(C)) + (4 \times C - (H)_2(C)(C_d)) + (1 \times 1,5$ -Cyclooctadiene rsc) Spiropentane $(4 \times C - (H)_2(C)_2) + (1 \times C - (C)_4) + (1 \times Spiropentane rsc)$	59STU/WES
Liquid Phase $\Delta_t H^\circ = 69.70 69.70 0.00 89STE/CHI$ $C_\rho^\circ = 145.94 145.94 0.00 76GEI/WOL$ $\Delta_t S^\circ = 189.37 189.37 0.00 76GEI/WOL$ $\Delta_t G^\circ = 179.23 S^\circ = 220.29 220.29 0.00 4$ $\Delta_t G^\circ = 179.23 \Delta_t S^\circ = -347.91$ $\Delta_t G^\circ = 358.24 10K_t = -144.51$ $1,5$ -Cyclooctadiene $(4 \times C_\sigma - (H)(C)) + (4 \times C - (H)_2(C)(C_d)) + (1 \times 1,5$ -Cyclooctadiene rsc) $(4 \times C_\sigma - (H)_2(C)_2) + (1 \times C - (C)_4) + (1 \times Spiropentane rsc)$	
Liquid Phase $ \Delta_t H^\circ = \begin{array}{ccccccccccccccccccccccccccccccccccc$	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
$C_{\rho}^{\circ} = 145.94 145.94 0.00 76GEI/WOL $ Liquid Phase $S^{\circ} = 189.37 189.37 0.00 76GEI/WOL $ $\Delta_{t}S^{\circ} = -367.35 C_{\rho}^{\circ} = 185.18 185.18 0.00 4$ $C_{\rho}^{\circ} = 185.18 185.18 0.00 4$ $S^{\circ} = 220.29 220.29 0.00 4$ $C_{\rho}S^{\circ} = 220.29 220.29 0.00 4$ $C_{\rho}S^{\circ} = -347.91 C_{\rho}S^{\circ} = -347.91 C_{$	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	TODO GOOT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	SOPRO/JOH
$ \frac{\ln K_f = -72.30}{\Delta_t G^\circ = 358.24} $ $ \frac{\ln K_f = -144.51}{\ln K_f = -144.51} $ $ \frac{(4 \times C_d - (H)(C)) + (4 \times C - (H)_2(C)(C_d)) + (1 \times 1,5 - Cyclooctadiene rsc)}{(1 \times 1,5 - Cyclooctadiene rsc)} $ $ \frac{\text{Spiropentane}}{(4 \times C_d - (H)_2(C)_2) + (1 \times C_d - (C)_d) + (1 \times Spiropentane rsc)} $	19SCO/GRO
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	19SCO/GRO
1,5-Cyclooctadiene C_8H_{12}	
1,5-Cyclooctadiene C_8H_{12} $(4 \times C_d - (H)(C)) + (4 \times C_d - (H)_2(C)(C_d)) + (1 \times 1,5$ -Cyclooctadiene rsc) Spiropentane $(4 \times C_d - (H)_2(C)_2) + (1 \times C_d - (C)_4) + (1 \times Spiropentane rsc)$	
$(4 \times C_d - (H)(C)) + (4 \times C - (H)_2(C)(C_d)) + (1 \times 1,5 - Cyclooctadiene rsc)$ $Spiropentane$ $(4 \times C - (H)_2(C)_2) + (1 \times C - (C)_4) + (1 \times Spiropentane rsc)$	
$(4 \times C - (H)_2(C)_2) + (1 \times C - (C)_4) + (1 \times Spiropentane rs$	C ₅ H ₆
Literature - Calculated = Residual Reference	
	Reference
Gas Phase	
$\Delta_t H^{\circ} = 101.10$ 101.10 0.00 76KOZ/TIM Gas Phase $\Delta_t H^{\circ} = 185.18$ 185.18 0.00 5	OSCO/EINO
	SOSCO/FIN2
	SOSTU/WES
•	9STU/WES
$S^{\circ} = 264.35$ 264.35 0.00 75LEB/TSV $\ln K_f = -107.03$ $\Delta_t S^{\circ} = -565.00$	
$\Delta_{i}G^{\circ} = -505.00$ $\Delta_{i}G^{\circ} = 226.15$	
$\ln K_f = -91.23$	

Spiropentan (4×C-(H	te (Continue $(C)_2(C)_2$) + $(1)_2(C)_2$	ed) ×C-(C) ₄)+(1:	× Spiropenta	C_5H_8 ne rsc), $\sigma = 4$			\times C-(H) ₂ (C) ₂)	+ (1 × C-(H)(C ₆ H ₁ (C) ₃) +
	Literature	e – Calculated =	= Residual	Reference	(1 × Cych		re – Calculated	== Residual	Reference
riid Dhaa								- Acoldulai	Reference
Liquid Phas $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{2}$	157.65 134.52 193.68	157.65 134.52 193.68 - 357.30 264.18 - 106.57	0.00 0.00 0.00	55FRA/PRO 50SCO/FIN2 50SCO/FIN2	Liquid Pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	se 58.95	-48.66 168.86 240.41 -577.46 123.51 -49.82	- 10.29	74GOO/MOO
		×C _d -(H) ₂)+(1	$1 \times C_d - (C)_2$	C ₅ H ₈	Methylcycle	opentane			C₅H _{1:}
	Literature	e – Calculated =	= Residual	Reference	(1×C-(H (1×-CH	$H_{3}(C)$) + (4) G_{3} corr (terti	\times C-(H) ₂ (C) ₂) (ary) + (ary) rsc), $\sigma =$		
Gas Phase $\Delta_l H^\circ = C_p^\bullet =$	121.55	119.46 85.81	2.09	74GOO/MOO		Literatui	re – Calculated	= Residual	Reference
Liquid Phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	93.85 131.13 210.20	90.36 132.17 204.98 - 346.00 193.52 - 78.07	3.49 -1.04 5.22	74GOO/MOO 81FIN/MES 81FIN/MES	Gas Phase $ \Delta_{t}H^{\circ} = C_{t}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = $	- 106.03 109.79 339.91	- 108.66 109.50 339.62 - 478.25 33.93 - 13.69	2.63 0.29 0.29	47OSB/GIN 69STU/WES 69STU/WES
	H) ₃ (C))+(3: obutane rsc)	× C-(H) ₂ (C) ₂) +) + (1 × -CH ₃ co c – Calculated -	orr (tertiary))	C ₅ H ₁₀ C) ₃)+	Liquid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se 137.74 158.70 247.78	- 133.89 156.22 245.58 - 572.29 36.74 - 14.82	-3.85 2.48 2.20	69GOO/SMI 46DOU/HUF2 46DOU/HUF2
Gas Phase $\Delta_t H^\circ = C_p^\circ =$		3.31 95.14				H) ₂) + (2 × 0	C-(H) ₂ (C) ₂)+(C_6H_{10}
Liquid Phase $\Delta_t H^\circ = C_p^\circ =$	se -44.48	-25.11 138.44	- 19.37	50HUM/SPI		Literatur	e – Calculated	= Residual	Reference
$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$		208.03 - 473.52 116.07 - 46.82			Gas Phase $\Delta_t H^\circ = C_p^\circ =$	12.01	6.99 95.65	5.02	75YUR/KAB
	H) ₃ (C))+(4: obutane rsc)	× C-(H) ₂ (C) ₂) + e – Calculated =		C ₆ H ₁₂ C) ₃)+ Reference	Liquid Phase $\Delta_{i}H^{\circ} = C^{\circ}_{p} = S^{\circ} = \Delta_{i}S^{\circ} = \Delta_{i}G^{\circ} = 0$	se 20.08	-18.42 147.69 241.11 -446.18 114.61	-1.66	61LAB/ROS
Gas Phase $\Delta_l H^\circ = C_p^\circ =$	-26.32	- 15.06 118.03	-11.26	74GOO/MOO	$lnK_f =$		-46.23		

TABLE 12. Cyclic CH-01 (40) - Continued

(2×-CH	corr (quat	\times C-(H) ₂ (C) ₂) -		C ₇ H ₁₄ +	trans-1,2-I (2×C-((2×-CF (1×Cyc	+ (2 × C-(H)(С ₇ H ₁₄ H)(С) ₃) +		
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas Phase	ı				Liquid Ph	ase			
$\Delta_{\rm f}H^{\circ} =$	-138.24	-137.41	-0.83	86TRC	$\Delta_{\rm f}H^{\circ} =$	- 171.21	-162.72	- 8.49	49JOH/PRO
$C_p^{\circ} =$	133.30	131.68	1.62	69STU/WES	$C_p^o =$	187.40	183.66	3.74	53GRO/OLI
S° =	359.28	356.15	3.13	69STU/WES	S° =	269.90	272.61	- 2.71	53GRO/OLI
$\Delta_f S^\circ =$		- 598.03		89.	$\Delta_{f}S^{\circ} =$		- 681.57		
$\Delta_f G^\circ = \ln K_f =$		40.89 16.50		.,	$\Delta_f G^\circ = \ln K_f =$		40.49 16.33		
			*****				·		·····
Liquid Pha				,		Dimethylcycl	-		С7Н
$\Delta_i H^\circ =$	-172.05	- 165.34	-6.71	49JOH/PRO	•		\times C-(H) ₂ (C) ₂)	$+(2\times C-(H)($	C) ₃) +
$C_p^{\circ} =$	187.36	181.56	5.80	53GRO/OLI	•	H ₃ corr (tert	• //	40	
$S^{\circ} - \Delta_f S^{\circ} =$	265.01	254.12 - 700.06	10.89	53GRO/OLI	(1×Cyc	uopentane (sub) rsc), $\sigma =$	15	
$\Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} =$		- 700.06 43.38				Literatu	re – Calculated	= Residual	Reference
$\ln K_{\rm f} =$		- 17.50			-			- Residuai	
	, <u></u>				Gas Phase	;			
cis -1,2-Dim	ethylcyclop	entane		C7H14	$\Delta_t H^\circ =$	- 133.55	-133.72	0.17	86TRC
		\times C-(H) ₂ (C) ₂)	+ (2 × C-(H)(C) ₃) +	$C_p^{\circ} =$	134.47	132.42	2.05	69STU/WES
	l3 corr (tert				s° -	366.81	359.28	7.53	69STU/WES
(1 × Cycl	opentane ($sub) rsc), \sigma =$	18		$\Delta_{\rm f}S^{\circ} =$		-594.90		
					$\Delta_{\mathbf{f}}G^{\circ} =$		43.65		
	Literatu	re – Calculated	= Residual 	Reference	$lnK_f =$		– 17.61		
Gas Phase					Liquid Ph	ase			
$\Delta_i H^\circ =$	- 129.49	-133.72	4.23	86TRC	$\Delta_{\mathbf{f}}H^{\circ} =$	-168.07	-162.72	-5.35	49JOH/PRO
$C_p^{\circ} =$	134.14	132.42	1.72	69STU/WES	$C_p^{\circ} =$	189.32	183.66	5.66	53GRO/OLI
S° =	366.14	359.28	6.86	69STU/WES	S° =	271.54	272.61	- 1.07	53GRO/OLI
$\Delta_t S^\circ =$		- 594.90			$\Delta_{\mathbf{f}}S^{\circ} =$		-681.57		
$\Delta_i G^{\circ} =$		43.65			$\Delta_{\mathbf{f}}G^{\circ} =$		40.49		
lnK _f =		- 17.61 			lnK _f =		- 16.33		
Liquid Pha	nse				Ethylcyclo	pentane			C ₇ H ₁
$\Delta_i H^\circ =$	-165.27	- 162.72	-2.55	49JOH/PRO		-	\times C-(H) ₂ (C) ₂)	+ (1 × C-(H)(
$C_p^{\circ} =$	188.74	183.66	5.08	53GRO/OLI	(1×Cyc	lopentane (s	sub) rsc), $\sigma =$	3	
S° =	269.16	272.61	-3.45	53GRO/OLI					
		- 681.57				Literatu	re – Calculated	= Residual	Reference
$\Delta_t S^\circ =$		40.49							
$\Delta_t G^\circ =$		- 16.33			G 71				
$\Delta_t G^\circ = $ $\ln K_t = $					Gas Phase		107.00	0.00	OCT DC
$\Delta_f G^\circ =$					$\Delta_t H^{\circ} =$	- 126.94	-127.03	0.09	86TRC 69STU/WES
$\Delta_{f}G^{\circ} = \frac{\ln K_{f}}{-1}$	imethylcycl	opentane		C7H14		12176			
$\Delta_t G^\circ = \ln K_t = \frac{1}{2}$		•	+ (2×C-(H)(C ₇ H ₁₄ C) ₃) +	$C_p^{\circ} =$	131.75	132.39	- 0.64 - 0.46	
$\Delta_{f}G^{\circ} = \frac{\ln K_{f}}{\ln K_{f}} = \frac{1}{2 \times C - (2 \times C - (2 \times C + C + C + C + C + C + C + C + C + C$		$3 \times C - (H)_2(C)_2$	+ (2×C-(H)(S° =	131.75 378.32	378.78	-0.46	69STU/WES
$\Delta_{f}G^{\circ} = \frac{\ln K_{f}}{\ln K_{f}} = \frac{1}{2 \times C - (2 \times -C)}$	H) ₃ (C)) + (3 I ₃ corr (ter	$3 \times C - (H)_2(C)_2$			$S^{\circ} = \Delta_{f}S^{\circ} =$		378.78 - 575.40		
$\Delta_{l}G^{\circ} = \frac{\ln K_{l}}{\ln K_{l}} = \frac{1}{2 \times C - (2 \times -C)}$	H) ₃ (C)) + (3 I ₃ corr (ter	$3 \times C - (H)_2(C)_2$ siary)) +		C) ₃) +	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ}$		378.78 - 575.40 44.53		
$\Delta_{f}G^{\circ} = \frac{\ln K_{f}}{\ln K_{f}} = \frac{1}{2 \times C - (2 \times -C)}$	H) ₃ (C))+(3 I ₃ corr (teri lopentane ($3 \times C - (H)_2(C)_2$ siary)) +	18		$S^{\circ} = \Delta_{f}S^{\circ} =$		378.78 - 575.40		
$\Delta_t G^{\circ} = \frac{1}{\ln K_t} = \frac{1}{2} \text{trans -1,2-E}$ $(2 \times C - (1 \times Cyc)$	H) ₃ (C)) + (3 I ₃ corr (tert lopentane (Literatu	$3 \times C - (H)_2(C)_2$ $(G)_2(C)_2(C)_2(C)_2(C)_2(C)_2(C)_2(C)_2(C$	18	C) ₃) +	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \Delta_{f}G^{\circ} = InK_{f} = -$ Liquid Pha	378.32	378.78 - 575.40 44.53 - 17.96	- 0.46	69STU/WES
$\Delta_f G^\circ = \frac{1}{\ln K_f} = \frac{1}{2}$ trans -1,2-E (2 × C-() (2 × -CF) (1 × Cyc)	H) ₃ (C))+(3 H ₃ corr (terr lopentane (Literatu	$3 \times C - (H)_2(C)_2$ (ary) + (arc) + (arc) (arc) + (arc) + (arc) (arc) + (arc) + (arc) (arc) + (18 = Residual	C) ₃) + Reference	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = \frac{1}{2}$ Liquid Pha $\Delta_{f}H^{\circ} = \frac{1}{2}$	378.32 ase - 163.43	378.78 - 575.40 44.53 - 17.96	- 0.46 - 5.99	69STU/WES
$\Delta_t G^\circ = \ln K_t = \frac{1}{2}$ trans-1,2-E (2×C-(: (2×-CF) (1×Cyc) Gas Phase $\Delta_t H^\circ = \frac{1}{2}$	H) ₃ (C)) + (3 H ₃ corr (terrilopentane (Literature) -136.65	$3 \times C - (H)_2(C)_2$ (ary) + (b) + (b) (ary)	18 = Residual -2.93	C) ₃) + Reference 86TRC	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = InK_{f} = InK_{f} = InG^{\circ}$ Liquid Pha $\Delta_{f}H^{\circ} = C_{p}^{\circ} = InG^{\circ}$	378.32 ase - 163.43 185.31	378.78 -575.40 44.53 -17.96 -157.44 186.64	- 5.99 - 1.33	69STU/WES 46JOH/PRO 53GRO/OLI
$\Delta_t G^\circ = \ln K_t = \frac{1}{\ln K_t}$ $C^\circ = \ln K_t = \frac{1}{\ln K_t}$ $C^\circ = \frac{1}{\ln K_t}$ $C^\circ = \frac{1}{\ln K_t}$ $C^\circ = \frac{1}{\ln K_t}$ $C^\circ = \frac{1}{\ln K_t}$	H) ₃ (C)) + (: I ₃ corr (terilopentane (Literature – 136.65 134.47	$3 \times C - (H)_2(C)_2$ $(1) \times $	18 = Residual -2.93 2.05	Reference 86TRC 69STU/WES	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = -\frac{1}{2}$ Liquid Photo $\Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = -\frac{1}{2}$	378.32 ase - 163.43	378.78 -575.40 44.53 -17.96 -157.44 186.64 277.96	- 0.46 - 5.99	69STU/WES 46JOH/PRO
$\Delta_t G^\circ = \ln K_t = \frac{1}{100}$ $\int_{0}^{\infty} \frac{1}{100} \int_{0}^{\infty} 1$	H) ₃ (C)) + (3 H ₃ corr (terrilopentane (Literature) -136.65	3×C-(H) ₂ (C) ₂) iary)) + sub) rsc), σ = re - Calculated -133.72 132.42 359.28	18 = Residual -2.93	C) ₃) + Reference 86TRC	$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = InK_f = InK_$	378.32 ase - 163.43 185.31	378.78 -575.40 44.53 -17.96 -157.44 186.64 277.96 -676.22	- 5.99 - 1.33	69STU/WES 46JOH/PRO 53GRO/OLI
$\Delta_t G^{\circ} = \frac{1}{\ln K_t} = \frac{1}{2}$ $trans \cdot 1, 2 \cdot \Gamma$ $(2 \times C - C)$ $(2 \times - C \cdot C)$ $(1 \times Cyc)$ $Gas \ Phase$ $\Delta_t H^{\circ} = C_{\rho}^{\circ} = C$	H) ₃ (C)) + (: I ₃ corr (terilopentane (Literature – 136.65 134.47	$3 \times C - (H)_2(C)_2$ $(1) \times $	18 = Residual -2.93 2.05	Reference 86TRC 69STU/WES	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = -\frac{1}{2}$ Liquid Photo $\Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = -\frac{1}{2}$	378.32 ase - 163.43 185.31	378.78 -575.40 44.53 -17.96 -157.44 186.64 277.96	- 5.99 - 1.33	69STU/WES 46JOH/PRO 53GRO/OLI

C10H20

TABLE 12. Cyclic CH-01 (40) - Continued

TABLE 13. Cyclic CH-02 (48)

	Literatur	e – Calculated	= Residual	Reference
Gas Phase	:			
$\Delta_{f}H^{\circ} =$	- 147.74	- 147.66	-0.08	47OSB/GIN
$C_p^{\circ} =$	154.64	155.28	-0.64	69STU/WES
S° =	417.27	417.94	-0.67	69STU/WES
$\Delta_f S^\circ =$		-672.55		
$\Delta_t G^\circ =$		52.86		
$lnK_{f} =$		-21.32		
Liquid Ph	ase			
$\Delta_{f}H^{\circ} =$	- 189.07	- 183.17	-5.90	46JOH/PRO
$C_p^{\circ} =$	216.27	217.06	-0.79	65MES/TOD2
S° =	310.83	310.34	0.49	65MES/TOD2
$\Delta_{c}S^{\circ} =$		-780.15		
$\Delta_i G^\circ =$		49.43		
		19.94		

,	(H)3(C))+(7	\times C-(H) ₂ (C) ₂) sub) rsc), $\sigma = 1$		C₉H ₁ (C) ₃) +
(27.0)	. `	re – Calculated		Reference
Gas Phase	;			
$\Delta_{\rm f}H^{\circ} =$	-168.28	- 168.29	0.01	69STU/WES
$C_{\rho}^{\circ} =$	177.49	178.17	- 0.68	69STU/WES
s° =	456.22	457.10	-0.88	69STU/WES
$\Delta_t S^\circ =$		- 769.70		
$\Delta_{\mathbf{f}}G^{\circ} =$		61.20		
lnK _f =		- 24.69		···
Liquid Ph	ase			
$\Delta_{f}H^{\circ} =$		-208.90		
$C_p^{\circ} =$	245.35	247.48	-2.13	65MES/TOD2
S° =	343.84	342.72	1.12	65MES/TOD2
$\Delta_f S^\circ =$		- 884.08		
$\Delta_f G^\circ =$		54.69		
$lnK_{\ell} =$		-22.06		

Pentylcyclopentane $(1 \times C - (H)_3(C)) + (8 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)_3) + (1 \times Cyclopentane (sub) rsc), \sigma = 3$

	Literatur	Reference		
Gas Phase	,			
$\Delta_t H^\circ =$	-188.91	-188.92	0.01	69STU/WES
$C_p^{\circ} =$	200.37	201.06	-0.69	69STU/WES
S° =	495.18	496.26	- 1.08	69STU/WES
$\Delta_f S^\circ =$		-866.85		
$\Delta_f G^\circ =$		69.53		
$lnK_f =$		-28.05		
Liquid Ph	ase			
$\Delta_{i}H^{\circ} =$		-234.63		
$C_p^{\circ} =$		277.90		
S° =		375.10		
$\Delta_f S^\circ =$		-988.01		
$\Delta_f G^\circ =$		59.95		
$lnK_f =$		-24.18		

Hexylcyclopentane $(1 \times C - (H)_3(C)) + (9 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)_3) + (1 \times Cyclopentane (sub) rsc), \sigma = 3$

	Literatu	Literature - Calculated = Residual			
Gas Phase	:				
$\Delta_{f}H^{\circ} =$	- 209.49	-209.55	0.06	69STU/WES	
$C_p^{\circ} =$	223.22	223.95	-0.73	69STU/WES	
S° =	534.13	535.42	- 1.29	69STU/WES	
$\Delta_f S^\circ =$		-964.01			
$\Delta_t G^{\circ} =$		77.87			
$\ln K_{\rm f} =$		-31.41			

TABLE 13. Cyclic CH-02 (48) - Continued

	pentane (Continued) $A_3(C) + (9 \times C - (H)_2(C)_2) + (9 \times C - (H)_2(C)_2) + (9 \times C)_2 + $	×C-(H)(0	$C_{11}H_{22}$ $C_{)3}) +$		- H)₃(C))+(1	$2 \times C - (H)_2(C)_2$ sub) rsc), $\sigma =$		C ₁₄ H (C) ₃) +
	Literature - Calculated = R	esidual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid Pha	se			Gas Phase				
$\Delta_{\mathbf{f}}H^{\circ} =$	-260.36			$\Delta_t H^{\circ} =$	-271.33	- 271.44	0.11	69STU/WES
$C_p^{\circ} =$	308.32			$C_p^{\circ} =$	291.83	292.62	-0.79	69STU/WES
S° =	407.48			<i>S</i> ° =	650.95	652.90	- 1.95	69STU/WES
$\Delta_f S^\circ =$	- 1091.94			$\Delta_{f}S^{\circ} =$		- 1255.46		
$\Delta_t G^\circ =$	65.20			$\Delta_t G^{\circ} =$		102.87		
$lnK_f =$	-26.30			$lnK_f =$		-41.50		
				Linuid Dha				
Hants-lawel	nontano		C H	Liquid Pha $\Delta_t H^\circ =$	iac .	_ 227 55		
Heptylcyck		(1 v C (T)	C ₁₂ H ₂₄			-337.55		
	$(H)_3(C) + (10 \times C - (H)_2(C)_2) + (10 \times C - (H)_2(C$	(1 × C-(H)	(C)3) T	$C_p^{\circ} = S^{\circ} =$		399.58		
(1 × Cyc	lopentane (sub) rsc), $\sigma = 3$					504.62		
	There are a control of		D - f -	$\Delta_t S^\circ =$		- 1403.73		
	Literature – Calculated = R	lesidual	Reference	$\Delta_{\rm f}G^{\circ} =$		80.97		
·				$\ln K_{\rm f} =$		- 32.66		
Gas Phase $\Delta_t H^\circ =$	-230.12 -230.18	0.06	69STU/WES					
$C_p^{\circ} =$	246.10 246.84	-0.74	69STU/WES	Decylcyclop	nentane			СИ
$S^{\circ} =$	573.04 574.58	-0.74	69STU/WES			3×C-(H) ₂ (C) ₂) (1×C (H)	C ₁₅ H
	-1061.16	-1.54	09310/WE3					(C)3) T
$\Delta_f S^\circ =$				(1 x Cyci	openiane (s	sub) rsc), σ =	3	
$\Delta_{\mathbf{f}}G^{\circ} =$	86.20				.			
$lnK_f =$	-34.77 				Literatui	re – Calculated	= Kesidual	Reference
Liquid Pha	ISE			Gas Phase				
$\Delta_i H^\circ =$	- 286.09			$\Delta_f H^\circ =$	- 292.33	- 292.07	-0.26	86TRC
$C_p^{\circ} =$	338.74			C_p° -	314.72	315.51	- 0.20 - 0.79	69STU/WES
$S^{\circ} =$	439.86			$S^{\circ} =$	689.90	692.06	-2.16	69STU/WES
$\Delta_f S^\circ =$	- 1195.87			Δ ₁ S° =	009.90	- 1352.61	-2.10	0931 O/ WES
				$\Delta_{\rm f}G^{\circ} =$				
$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{I}} =$	70.46 28.42			$\ln K_{\rm f} -$		111.21 44.86		
				T : . : 1 Pl				
			C 17	Liquid Pha		- 363.28	-4.70	55FRA/PRO2
Λ-4-1I							-4.70	JJI KAVI KUL
		(1 v C (U)	C ₁₃ H ₂₆	$\Delta_t H^\circ -$	- 367.98			
(1×C-($(H)_3(C) + (11 \times C - (H)_2(C)_2) +$	(1×C-(H)		$C_p^{\alpha} =$	- 307.90	430.00		
(1×C-((1×C-(H)		$C_p^{\circ} = S^{\circ} =$	- 307.96	430.00 537.00		
(1×C-(H) ₃ (C)) + (11 × C-(H) ₂ (C) ₂) + lopentane (sub) rsc), $\sigma = 3$		(C)₃)+	$C_p^\circ = S^\circ = \Delta_t S^\circ =$	- 307.96	430.00 537.00 -1507.66		
(1×C-($(H)_3(C) + (11 \times C - (H)_2(C)_2) +$			$C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \Delta_t G^{\circ} = \Delta_t G^{\circ} = 0$	- 367.96	430.00 537.00 -1507.66 86.23		
	H) ₃ (C)) + (11 × C-(H) ₂ (C) ₂) + lopentane (sub) rsc), $\sigma = 3$		(C)₃)+	$C_p^\circ = S^\circ = \Delta_t S^\circ =$	- 301.90	430.00 537.00 -1507.66		
(1 × C-((1 × Cyc	H) ₃ (C)) + $(11 \times C - (H)_2(C)_2)$ + lopentane (sub) rsc), $\sigma = 3$ Literature — Calculated — F	Cosidual	(C) ₃)+ Reference	$C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \Delta_t G^{\circ} = \Delta_t G^{\circ} = 0$	- 301.90	430.00 537.00 -1507.66 86.23		
(1×C-((1×Cyc Gas Phase Δ _t II° -	H) ₃ (C)) + $(11 \times C - (H)_2(C)_2)$ + lopentane (sub) rsc), $\sigma = 3$ Literature – Calculated – F -250.71 –250.81	0.10	(C) ₃) + Reference 69STU/WES	$C_p^o = S^o = S^o = \Delta_f S^o = \Delta_f G^o = \ln K_f =$		430.00 537.00 -1507.66 86.23 -34.78	***************************************	
$(1 \times C - (1 \times Cyc) + Cyc)$ Gas Phase $\Delta_t II^\circ - C_p^\circ =$	H) ₃ (C)) + (11 × C-(H) ₂ (C) ₂) + lopentane (sub) rsc), $\sigma = 3$ Literature – Calculated – F -250.71 –250.81 268.99 269.73	0.10 - 0.74	(C) ₃) + Reference 69STU/WES 69STU/WES	$C_p^o = S^o = S^o = \Delta_f S^o = \Delta_f G^o = \ln K_f =$	cyclopentane	430.00 537.00 -1507.66 86.23 -34.78		C ₇ H ₁
$(1 \times C - (1 \times Cyc))$ Gas Phase $\Delta_t II^\circ - C_t^\circ = S^\circ = S$	H) ₃ (C)) + (11 × C-(H) ₂ (C) ₂) + lopentane (sub) rsc), $\sigma = 3$ Literature – Calculated – F -250.71 – 250.81 268.99 269.73 611.99 613.74	0.10	(C) ₃) + Reference 69STU/WES	$C_p^o = S^o = S^o = \Delta_t S^o = \Delta_t G^o \sim \ln K_t =$ Ethylidened	cyclopentan	430.00 537.00 -1507.66 86.23 -34.78		
Gas Phase $\Delta_t II^{\circ} - C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} =$	H) ₃ (C)) + (11 × C-(H) ₂ (C) ₂) + lopentane (sub) rsc), $\sigma = 3$ Literature – Calculated – F -250.71 –250.81 268.99 269.73 611.99 613.74 –1158.31	0.10 - 0.74	(C) ₃) + Reference 69STU/WES 69STU/WES	$C_p^o = S^o = S^o = \Delta_t S^o = \Delta_t S^o = \Delta_t C^o \sim \ln K_t = \frac{1}{2}$ Ethylidenec	cyclopentano $S(C) + (1 \times 1)$	430.00 537.00 -1507.66 86.23 -34.78		C ₇ H ₁ (4×C-(H) ₂ (C) ₂)
$(1 \times C - (1 \times Cyc))$ Gas Phase $\Delta_t II^\circ - C_t^\circ = S^\circ = S$	H) ₃ (C)) + (11 × C-(H) ₂ (C) ₂) + lopentane (sub) rsc), $\sigma = 3$ Literature – Calculated – F -250.71 – 250.81 268.99 269.73 611.99 613.74	0.10 - 0.74	(C) ₃) + Reference 69STU/WES 69STU/WES	$C_p^o = S^o = S^o = \Delta_t S^o = \Delta_t S^o = \Delta_t C^o \sim \ln K_t = \frac{1}{2}$ Ethylidenec	cyclopentano $S(C) + (1 \times 1)$	430.00 537.00 -1507.66 86.23 -34.78		
Gas Phase $\Delta_t II^\circ - C_p^\circ = S^\circ = \Delta_t S^\circ =$	H) ₃ (C)) + (11 × C-(H) ₂ (C) ₂) + lopentane (sub) rsc), $\sigma = 3$ Literature – Calculated – F -250.71 –250.81 268.99 269.73 611.99 613.74 –1158.31	0.10 - 0.74	(C) ₃) + Reference 69STU/WES 69STU/WES	$C_p^o = S^o = S^o = \Delta_t S^o = \Delta_t S^o = \Delta_t C^o \sim \ln K_t = \frac{1}{2}$ Ethylidenec	cyclopentane (C)) + (1×0) + (1×0)	430.00 537.00 -1507.66 86.23 -34.78	b) rsc)	
Gas Phase $ \Delta_t H^\circ - C_p^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	H) ₃ (C)) + (11 × C-(H) ₂ (C) ₂) + lopentane (sub) rsc), $\sigma = 3$ Literature – Calculated – F - 250.71 – 250.81 268.99 269.73 611.99 613.74 - 1158.31 94.54 - 38.14	0.10 - 0.74	(C) ₃) + Reference 69STU/WES 69STU/WES	$C_p^o = S^o = S^o = \Delta_t S^o = \Delta_t S^o = \Delta_t C^o \sim \ln K_t = \frac{1}{2}$ Ethylidenec	cyclopentane (C)) + (1×0) + (1×0)	430.00 537.00 -1507.66 86.23 -34.78	b) rsc)	(4×C-(H) ₂ (C) ₂)
Gas Phase $\Delta_t II^{\circ} - C_p^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = $ Liquid Pha $\Delta_t H^{\circ} = C_t^{\circ} = C_t^{\circ} = C_t^{\circ}$	H) ₃ (C)) + (11 × C-(H) ₂ (C) ₂) + lopentane (sub) rsc), $\sigma = 3$ Literature – Calculated – F - 250.71 – 250.81 268.99 269.73 611.99 613.74 - 1158.31 94.54 - 38.14	0.10 - 0.74	(C) ₃) + Reference 69STU/WES 69STU/WES	$C_p^o = S^o = S^o = \Delta_t S^o = \Delta_t S^o = \Delta_t C^o \sim \ln K_t = \frac{1}{2}$ Ethylidenec	cyclopentane (C)) + (1×0) + (1×0)	430.00 537.00 -1507.66 86.23 -34.78	b) rsc)	(4×C-(H) ₂ (C) ₂)
Gas Phase $\Delta_{t}H^{\circ} - C_{p}^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = $ Liquid Pha	H) ₃ (C)) + (11 × C-(H) ₂ (C) ₂) + lopentane (sub) rsc), $\sigma = 3$ Literature – Calculated – F - 250.71 – 250.81 268.99 269.73 611.99 613.74 - 1158.31 94.54 - 38.14	0.10 - 0.74	(C) ₃) + Reference 69STU/WES 69STU/WES	$C_p^o = S^o = S^o = \Delta_t $	cyclopentane (C)) + (1×0) + (1×0)	430.00 537.00 -1507.66 86.23 -34.78	b) rsc)	(4×C-(H) ₂ (C) ₂)
Gas Phase $\Delta_t II^{\circ} - C_p^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = $ Liquid Pha $\Delta_t H^{\circ} = C_t^{\circ} = C_t^{\circ} = C_t^{\circ}$	H) ₃ (C)) + (11 × C-(H) ₂ (C) ₂) + lopentane (sub) rsc), $\sigma = 3$ Literature – Calculated – F - 250.71 – 250.81 268.99 269.73 611.99 613.74 - 1158.31 94.54 - 38.14 ase - 311.82	0.10 - 0.74	(C) ₃) + Reference 69STU/WES 69STU/WES	$C_p^o = S^o = S^o = \Delta_t $	cyclopentane (C)) + (1×0) + (1×0)	430.00 537.00 -1507.66 86.23 -34.78 C _d -(H)(C))+(1 clopentane (sul	b) rsc)	(4×C-(H) ₂ (C) ₂)
$(1 \times C - (1 \times Cyc))$ Gas Phase $\Delta_t II^{\circ} - C_p^{\circ} = S_p^{\circ} = \Delta_t S^{\circ} = \ln K_t = 1$ Liquid Pha $\Delta_t H^{\circ} = C_p^{\circ} = 1$	H) ₃ (C)) + (11 × C-(H) ₂ (C) ₂) + lopentane (sub) rsc), $\sigma = 3$ Literature - Calculated - F - 250.71 - 250.81 268.99 269.73 611.99 613.74 - 1158.31 94.54 - 38.14 ase - 311.82 369.16	0.10 - 0.74	(C) ₃) + Reference 69STU/WES 69STU/WES	$C_p^o = S^o = S^o = \Delta_t S^o = \Delta_t S^o = \Delta_t C^o = \ln K_t = \frac{1}{2}$ Ethylidenee (1×C-(H):	cyclopentane (C)) + (1×0) + (1×0)	430.00 537.00 -1507.66 86.23 -34.78 C _d -(H)(C))+(1 clopentane (sul re-Calculated	b) rsc)	(4×C-(H) ₂ (C) ₂)
Gas Phase $\Delta_{f} I^{\circ} - C_{p}^{\circ} = S^{\circ} = \Delta_{f} S^{\circ} = \ln K_{f} = \lim_{K \to \infty} \Delta_{f} H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \lim_{K \to \infty} \Delta_{f} H^{\circ} = G^{\circ} = S^{\circ} = \lim_{K \to \infty} \Delta_{f} H^{\circ} = G^{\circ} = S^{\circ} = \lim_{K \to \infty} \Delta_{f} H^{\circ} = G^{\circ} = G^{\circ$	H) ₃ (C)) + (11 × C-(H) ₂ (C) ₂) + lopentane (sub) rsc), $\sigma = 3$ Literature - Calculated - F -250.71 -250.81 268.99 269.73 611.99 613.74 -1158.31 94.54 -38.14 ase -311.82 369.16 472.24	0.10 - 0.74	(C) ₃) + Reference 69STU/WES 69STU/WES	$C_p^o = S^o = S^o = \Delta_t $	cyclopentane (C)) + (1×0) + (1×0)	430.00 537.00 -1507.66 86.23 -34.78 C _d -(H)(C))+(1 clopentane (sul re-Calculated	b) rsc)	(4×C-(H) ₂ (C) ₂)

TABLE 13	. Cyclic	CH-02	(48)	_	Continued
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TABLE 13. Cyclic CH-02 (48) - Continued

Ethylidenecyclopentan		C (C)) ·	C ₇ H ₁₂		$H_{2}(C)_{2}+C$	2×C-(H)(C) ₃)	+	C ₁₀ H
(1×C-(H)₃(C))+(1× + (1×C)	C_d -(H)(C))+(1× α clopentane (sub) 1		(4×C-(H) ₂ (C) ₂)	(2×Cycle	opentane (s Literatur	sub) rsc) re – Calculated	= Residual	Reference
Literatu	re – Calculated = R	Residual	Reference					
				Gas Phase $\Delta_t H^\circ =$		- 128.28		
Liquid Phase $\Delta_t H^\circ = -56.74$	-56.73	-0.01	61LAB/ROS	$C_{\rho}^{\circ} =$		167.54		
$C_p^{\circ} = 181.17$	182.66	-1.49	79FUC/PEA			107.54		
S° =	268.22							
$\Delta_{f}S^{\circ} =$	-555.39			Liquid Pha				
$\Delta_t G^\circ =$	108.86			$\Delta_{f}H^{\circ} =$	-179.33	- 168.20	-11.13	76GOO/LEE
$lnK_f =$	-43.91			$C_p^{\circ} =$	238.91	239.48	-0.57	76GOO/LEE
				S° =		324.56		
				$\Delta_f S^\circ =$		-907.98		
Ethenylcyclopentane			C ₇ H ₁₂	$\Delta_f G^\circ = \ln K_f =$		102.51 41.35		
$(1 \times C_d - (H)_2) + (1 \times C_d - (H)_2(C)_2) +$		sub) rsc)	(C _d))+ Reference	1-Methylcyc	clopentene			Cel
						$\times C_{d}$ -(C) ₂)+(1+(1×C-(H) ₂)	C/-/+ C/-/+	
Gas Phase						$\tau(1 \wedge C - (11)_2($ sub) rsc), $\sigma =$		
$\Delta_t H^\circ =$	-1.96			(17. C)Cit	opontono (d	130), 0	-	
C _p =	131.30				Literatu	re – Calculated	= Residual	Reference
Liquid Phase				Gas Phase				
$\Delta_t H^\circ = -34.81$	-31.55	-3.26	61LAB/ROS	$\Delta_t H^\circ =$	-3.81	0.12	-3.93	79FUC/PEA
$C_p^{\circ} =$	181.45	5.20	OILI ID/NOU	$C_p^{\circ} =$	100.83	99.22	1.61	69STU/WES
S° =	272.87			S° =	326,35	333.07	-6.72	69STU/WES
$\Delta_f S^\circ =$	-550.74			$\Delta_{r}S^{\circ} =$		- 354.23	52	0,010,20
$\Delta_{f}G^{\circ} =$	132.65			$\Delta_{\mathbf{f}}G^{\circ} =$		105.73		
$lnK_f =$	- 53.51			$lnK_f =$		-42.65		
				Liquid Phas	se			
11-Cyclopentylheneico			$C_{26}H_{52}$	$\Delta_t H^{\circ} =$	-36.44	- 34.77	-1.67	69GOO/SMI
$(2 \times C - (H)_3(C)) + (2 \times C - (H)_3(C))$		(2×C-(H)	(C) ₃)+	$C_p^{\circ} =$	153.10	157.48	-4.38	79FUC/PEA
(1×Cyclopentane (sub) rsc)			S° =		226.14		
- •			~ .	$\Delta_{\rm f}S^{\circ} =$		-461.15		
Literatu	re – Calculated = R	Residual	Reference	$\Delta_t G^{\circ} =$		102.72		
				$lnK_f =$		-41.44		
Gas Phase	501 17							
$\Delta_{\mathbf{f}}H^{\circ} =$	-521.17			2 Madeal				~
$C_p^{\circ} =$	567.33			3-Methylcyc		v С_(II) (С)(С	1.)) ± (1 × 0 · 0	C ₆ H ₁
						×С-(H)₂(С)(С ×С-(H)(С)₂(С	(C_d)) + (1 × C-(H	1/2(0/2)+
					corr (terti		(d)) T	
Liquid Phase		- 1.29	44KNO/HUF			ub) rsc), $\sigma = 0$	3	
	- 647.23			(20)	L (9		-	
$\Delta_i H^\circ = -648.52$	- 647.23 761.64							D . C
$\Delta_t H^\circ = -648.52$ $C_p^\circ = S^\circ =$	-647.23 761.64 887.83				Literatur	e – Calculated	= Residual	Reference
$\Delta_t H^\circ = -648.52$ $C_p^\circ =$	761.64				Literatur	e – Calculated	= Residual	Keterence
$\Delta_t H^\circ = -648.52$ $C_p^\circ = S^\circ = \Delta_t S^\circ =$	761.64 887.83				Literatur	e – Calculated	= Residual	Keterence
$\Delta_{t}H^{\circ} = -648.52$ $C_{p}^{\circ} = S^{\circ} =$	761.64 887.83 2656.26			Gas Phase	Literatur	e – Calculated	= Residual 	Keterence
$\Delta_{i}H^{\circ} = -648.52$ $C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = S^{\circ} =$	761.64 887.83 2656.26 144.73			$\Delta_{\ell}H^{\circ} =$	7.36	9.29	= Residual 	79FUC/PEA
$\Delta_{i}H^{\circ} = -648.52$ $C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = S^{\circ} =$	761.64 887.83 2656.26 144.73			$ \Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = $				
$\Delta_{s}H^{\circ} = -648.52$ $C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = S^{\circ} =$	761.64 887.83 2656.26 144.73			$\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} =$	7.36	9.29 109.72 328.38	- 1.93	79FUC/PEA
$\Delta_{i}H^{\circ} = -648.52$ $C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = S^{\circ} =$	761.64 887.83 2656.26 144.73			$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	7.36 100.00	9.29 109.72 328.38 -358.92	- 1.93 - 9.72	79FUC/PEA 69STU/WES
$C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = $	761.64 887.83 2656.26 144.73			$\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} =$	7.36 100.00	9.29 109.72 328.38	- 1.93 - 9.72	79FUC/PEA 69STU/WES

TABLE 13. Cyclic CH-02 (48) - Continued

(2×C _d -(I (1×C-(H	$(1)_3(C) + (1)$	< C-(H) ₂ (C)(C _d < C-(H)(C) ₂ (C _d		C_6H_{10} $H_{12}(C)_2) +$		$H_{3}(C)) + (1$	×C-(H)(C) ₃) + l ×Cyclohexane		
	, corr (tertia ppentene (su	(ry)) + (rsc) , $\sigma = 3$				Literatu	re – Calculated	= Residual	Reference
	Literature	- Calculated =	Residual	Reference					
					Gas Phase $\Delta_t H^\circ =$	154.70	140.00	5.40	47OCD CIN
Liquid Phas	se.				$C_p^{\circ} =$	- 154.72 135.02	- 149.23 137.44	- 5.49 - 2.42	47OSB/GIN 69STU/WES
$\Delta_t H^\circ =$	- 23.68	-24.35	0.67	61LAB/ROS	S° =	343.34	344.36	-1.02	69STU/WES
$C_p^{\circ} =$		159.69			$\Delta_{f}S^{\circ} =$		-609.82		
S° =		224.81		• 1	$\Delta_{\rm f}G^{\circ} =$		32.59		
$\Delta_f S^\circ =$		- 462.48		•	$lnK_f =$		- 13.15		
$\Delta_{\rm f}G^{\circ} =$		113.54							
$\ln K_{\rm f} =$		-45.80		1	Liquid Pha	se.			
			····		$\Delta_t H^\circ =$	- 190.08	- 185.27	-4.81	46JOH/PRO
					$C_p^{\circ} =$	184.51	183.75	0.76	46DOU/HUF2
4-Methylcyc	lopentene			C ₆ II ₁₀	S° -	247.90	246.41	1.49	46DOU/HUF2
(2×C _d -(H)(C))+(2:	\times C-(H) ₂ (C)(C _c	$(1 \times C - (1 \times C - (1 \times C + (1 \times C) + ($	H) ₃ (C))+	$\Delta_i S^\circ =$		-707.77		
		×-CH ₃ corr (te			$\Delta_{\mathbf{f}}G^{\circ} =$		25.75		
(1 × Cycle		ub) rsc), σ = 3 e – Calculated =		Reference	$lnK_f =$		- 10.39		
	Literatur	Calculated -	residual						
							yclopentyl-1-pro	-	C ₈ H ₁₄
Gas Phase							C_d – $(H)(C))+(1$		(C _d))+
$\Delta_t H^\circ =$	14.77	9.50	5.27	69STU/WES			× C-(H) ₂ (C) ₂)	+	
$C_{\rho}^{\circ} = S^{\circ} =$	100.00 328.86	100.05	0.05 4.66	69STU/WES	(1 × Cycl	opentane (s	sub) rsc)		
$\Delta_{f}S^{\circ} =$	320.00	324.20 - 363.10	4.00	69STU/WES		Litorotus	re – Calculated :	- Decidual	Reference
$\Delta_{i}G^{\circ} =$		117.76				Literatur	e – Calculateu	- Residual	Reference
$lnK_f =$		-47.50							
				.,,	Gas Phase				
					$\Delta_{\mathbf{f}}H^{\circ} =$	-19.10	-22.38	3.28	79FUC/PEA
Liquid Pha					$C_p^{\circ} =$		144.52		
$\Delta_{\mathbf{f}}H^{\circ} =$	-17.57	-24.10	6.53	61LAB/ROS					
$C_p^{\circ} =$		149.82			7 · · · · · Di				
S° = Δ _ι S° =		228.28 - 459.01			Liquid Phat $\Delta_t H^* =$	se 59.50	-57.03	- 2.47	71ROG/MCL
$\Delta_{t}G^{\circ} =$		112.76			$C_p^{\circ} =$	202.92	202.00	0.92	79FUC/PEA
$\ln K_{\rm f} =$		-45.48			S° =	202.72	308.72	0.72	MOGILA
mari —		45.40			$\Delta_{f}S^{\circ} =$		-651.20		
					$\Delta_{\mathbf{f}}G^{\circ} =$		137.12		
					$lnK_f =$		-55.32		
1-Ethylcycl				C_7H_{12}					
		\times C-(H) ₂ (C)(C ₄							~ **
(1 × C _d -((H)(C))+(1	$\times C_{\mathbf{d}}$ -(C) ₂) + (1	× Cyclopente	ne (sub) rsc)	Methylenec	•	C_{d} – $(C)_2$)+ $(2\times$	C-(III)-(C)(C	C ₇ H ₁₂
	Literatur	e – Calculated =	= Residual	Reference			$1 \times \text{Cyclohexane}$		IJ, ⊤
					, ,	T 14	0-11	Desident	D . C
Gas Phase						Literatur	e – Calculated :	= Kesidual	Reference
$\Delta_f H^\circ =$	19.75	- 20.76	1.01	79FUC/PEA					
$C_p^{\circ} =$		119.85			Gas Phase				
-					$\Delta_{\mathbf{f}}H^{\circ} =$	-25.23	-33.58	8.35	79FUC/PEA
Liquid Pha	150				$C_p^{\circ} =$		123.59		
$\Delta_i H^\circ =$	-58.28	-60.50	2.22	61LAB/ROS					
$C_n^{\circ} =$	188.28	-00.30 186.77	1.51	79FUC/PEA	Liquid Phas	se			
S° =	200120	257.81		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	$\Delta_f H^\circ =$	-61.30	- 69.80	8.50	63PAS/ALM
Δ _f S° =		-565.80			$C_p^{\circ} =$	177.40	175.22	2.18	79FUC/PEA
$\Delta_f G^\circ =$		108.19			S° =		241.94	0	
$lnK_f =$		-43.64			$\Delta_{\mathbf{f}}S^{\circ} =$		-581.67		
					$\Delta_t G^{\circ} =$		103.62		
					,		100.02		

1,1-Dimethy (2×C-(H (5×C-(H	$H_{3}(C)+(1$	ne ×C-(C) ₄) + (2 1 × Cyclohexan	×-CH ₃ corr (e (sub) rsc), o	C_aH_{16} (quaternary)) + $r = 9$	(2×C-($(H)_3(C)) + (2)$	lohexane (Cont 2×C-(H)(C) ₃) (1×Cyclohexan	+ (2×-CH ₃ c	C_8H_{16} orr (tertiary))+ $\sigma = 9$
	Literatu	re – Calculated	= Residual	Reference		Literatu	ire – Calculated	d = Residual	Reference
Gas Phase					Liquid Ph				
$\Delta_f H^\circ =$	- 180.87	177.98	-2.89	86TRC	$\Delta_{\rm f}H^{\circ} =$	-215.69	-214.10	1.59	47JOH/PRO2
$C_p^{\circ} =$	154.39	159.62	-5.23	69STU/WES	$C_p^{\circ} =$	212.84	211.19	1.65	49HUF/TOD
S° =	365.01	366.65	-1.64	69STU/WES	S° =	276.27	273.44	2.83	49HUF/TOD
$\Delta_t S^\circ =$		-723.84			$\Delta_f S^\circ = \Delta_f G^\circ =$		-817.05 29.50		
$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = $		37.83 - 15.26			$\ln K_{\rm f} =$		-11.90		
									
Liquid Pha $\Delta_t H^\circ =$	se -218.74	-216.72	-2.02	47JOH/PRO2	trans_1 4_T	Dimethylcycl	lohevane		CH
$\Delta_i H^{\circ} = C_p^{\circ} =$	209.24	209.09	0.15	49HUF/TOD				+ (2 × -CH, c	C ₈ H ₁₆ orr (tertiary))+
$S^{\circ} =$	267.23	254.95	12.28	49HUF/TOD			1 × Cyclohexan		
$\Delta_f S^\circ =$		-835.54			,,,,,			,	
$\Delta_t G^\circ = \ln K_t =$		32.40 13.07				Literatu	re – Calculated	l = Residual	Reference
		- 13.07			C Ph				
					Gas Phase $\Delta_t H^\circ =$	- 184.51	- 174.29	- 10.22	ATOCD/CIN
tname .1 2.Th	imethylcycl	ohevene		C ₈ H ₁₆	$C_p^{\circ} =$	157.74	160.36	- 10.22 - 2.62	47OSB/GIN 69STU/WES
		C×C-(H)(C)₃) +	+ (2 x - CH ₂ co		S° =	364.80	364.02	0.78	69STU/WES
		1 × Cyclohexane			$\Delta_f S^\circ =$		- 726.47	0.70	0,010,4123
()2()2) - (,	(),	-	$\Delta_{\rm f}G^{\circ} =$		42.31		
	Literatu	re – Calculated	= Residual	Reference	$lnK_t =$		-17.07		
Gas Phase	450.0 .	171.00	5.50	4500D (CINI	Liquid Pha		21.1.10	0.00	
$\Delta_i H^\circ =$	- 179.87 158.99	- 174.29 160.36	-5.58 -1.37	47OSB/GIN 69STU/WES	$\Delta_{f}H^{\circ} = C_{\rho}^{\circ} =$	- 222.38 210.25	-214.10	- 8.28	47JOH/PRO2
C; = S° =	370.91	369.78	1.13	69STU/WES	S° =	268.03	211.19 273.44	0.94 5.41	49HUF/TOD 47HUF/TOD
Δ _t S° =	370.71	- 720.71	1.13	0,010,1125	$\Delta_{f}S^{\circ} =$	200.05	-817.05	-3.41	4/1101/101
$\Delta_f G^\circ =$		40.59			$\Delta_{\rm f}G^{\circ} =$		29.50		
$lnK_f =$		- 16.37			$lnK_f =$		~11.90		
Liquid Pha	100								
$\Delta_i H^\circ =$	- 218.24	-214.10	-4.14	47JOH/PRO2	Ethylcyclol	hexane			C ₈ H ₁₆
$C_p^{\circ} =$	209.41	211.19	-1.78	49HUF/TOD			\times C-(H)(C) ₃)	+ (6×C-(H) ₂ (C)2)+
<i>S</i> ° =	273.22	273.44	-0.22	49HUF/TOD			ub) rsc), $\sigma = 3$		- /2/
$\Delta_f S^\circ =$		-817.05							
$\Delta_{\rm f}G^{\circ} =$		29.50				Literatu	re – Calculated	= Residual	Reference
$lnK_f =$		-11.90							
					Gas Phase $\Delta H^{\circ} =$	- 171.63	167.40	. 4.02	470en/013
trans -1.3-D	imethylcycl	ohexane		C ₈ H ₁₆	$C_p^{\circ} =$	158.82	167.60 160.33	- 4.03 - 1.51	47OSB/GIN 69STU/WES
		:×C-(H)(C)₃)+	F(2×−CH₂ co		S° =	382.58	383.52	-0.94	69STU/WES
		1 × Cyclohexane			$\Delta_f S^\circ =$	502.50	- 706.97	0.54	03310/1123
(,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,)2(-)2) . (•	$\Delta_t G^\circ =$		43.18		
	Literatu	re - Calculated	= Residual	Reference	$lnK_f =$		-17.42		
						· · · · · · · · · · · · · · · · · · ·			
Gas Phase		48			Liquid Pha			_	
$\Delta_i H^\circ =$	- 176.48	- 174.29	-2.19	47OSB/GIN	$\Delta_{\rm f}H^{\circ} =$	-212.13	- 208.82	-3.31	46JOH/PRO2
$C_p^{\circ} =$	157.32 376.33	160.36	-3.04	69STU/WES	$C_p^{\circ} =$	211.79	214.17	-2.38	49HUF/TOD
$S^{\circ} = \Delta_{t}S^{\circ} =$	376.23	369.78 720.71	6.45	69STU/WES	S° = Δ _t S° =	280.91	278.79	2.12	49HUF/TOD
$\Delta_t G^\circ =$		- 720.71 40.59			$\Delta_{\rm f}G^{\circ} =$		-811.70 33.19		
$\ln K_{\rm f} =$		- 16.37			$\ln K_{\rm f} =$		- 13.39		
mart -					maxt -		- 13.37		

TABLE 13. Cyclic CH-02 (48) - Continued

(1 × Cyclo		×C-(H)(C) ₃) + b) rsc), σ = 3		C ₃ H ₁₈ C) ₂)+	Pentylcyclohexane (Continued) $(1 \times C - (H)_3(C)) + (1 \times C - (H)(C)_3) + (9 \times C - (H)_2(C)_2) + (1 \times Cyclohexane (sub) rsc), \sigma = 3$				
	Literatur	e – Calculated	= Residual	Reference		Literature	e – Calculated	= Residual	Reference
Gas Phase				•	Liquid Phas	se			
$\Delta_f H^\circ =$	-192.30	- 188.23	-4.07	65FIN/MES	$\Delta_f H^\circ =$		-286.01		
$C_p^{\circ} =$	184.22	183.22	1.00	69STU/WES	$C_p^{\circ} =$		305.43		
S° =	419.53	422.68	-3.15	69STU/WES	S° =		375.93		
$\Delta_t S^\circ =$		-804.12			$\Delta_{\rm f} S^{\circ} =$		-1123.49		
$\Delta_f G^\circ = \ln K_f =$		51.52 - 20.78			$\Delta_f G^\circ = \ln K_f =$		48.96 19.75		
111VL -		- 20.76		anning that PP a TANK Section 1997			- 19.73		
Liquid Pha									
$\Delta_{\ell}H^{\circ} =$	-237.40	-234.55	-2.85	70GOO2	Dodecylcycl				C ₁₈ H
$C_p^{\circ} =$	242.04	244.59	-2.55	65FIN/MES	(1×C-(F	$I)_3(C)) + (1 \times 1)_3(C)$	< C-(H)(C) ₃) -	+ (16 × C-(H) ₂	₂ (C) ₂)+
S° =	311.88	311.17	0.71	65FIN/MES	(1 × Cyclo	ohexane (sut	o) rsc)		
$\Delta_{\rm f} S^{\circ} =$		-915.63				T :4	0-1-1	n	D. (
$\Delta_{\mathbf{f}}G^{\circ} = \ln K_{\mathbf{f}} =$		38.44 15.51				Literature	- Calculated	= Kesidual	Reference
				t transcor	Gas Phase				
						- 378.70	-373.90	-4.80	78FUC/PEA
Butylcycloh	exane			$C_{10}H_{20}$	$C_p^{\circ} =$		389.23		
		\times C-(H)(C) ₃)- b) rsc), $\sigma = 3$		C)₂)+	Liquid Phas				-
	Literatur	e – Calculated	= Residual	Reference	$\Delta_t H^\circ =$	467.56	-466.12 518.37	-1.44	40MOO/REN
					$C_p^\circ = S^\circ =$	615.50	602.59	12.91	49PAR/MOO
Gas Phase					$\Delta_f S^\circ =$		- 1851.01		•
$\Delta_{f}H^{\circ} =$	-213.10	-208.86	-4.24	65FIN/MES	$\Delta_t G^{\circ} =$		85.76		
$C_p^{\alpha} =$	207.11	206.11	1.00	69STU/WES	$lnK_f =$		- 34.59		
S° =	458.48	461.84	-3.36	69STU/WES					
$\Delta_f S^\circ =$	•	-901.27							
		£0.0£							
$\Delta_f G^{\circ} =$		59.85							
		59.85 24.15			1-Methylcyc (1×C-(H		< C _d (C) ₂) + (1	×-CH ₃ corr	C ₇ H ₁ (tertiary))+
$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = $					(1×C-(H (1×C _d -(l	I)₃(C))+(1× H)(C))+(2×	C-(H)2(C)(C	×-CH ₃ corr (C _d))+(2×C-(I	(tertiary))+
$\Delta_t G^\circ = \ln K_t =$ Liquid Pha		- 24.15	-2.81	46JOH/PRO2	(1×C-(H (1×C _d -(l	(1) ₃ (C))+(1×	C-(H)2(C)(C		(tertiary))+
$\Delta_t G^\circ = \ln K_t = $ Liquid Pha $\Delta_t H^\circ = $	use 263.09 271.04		-2.81 -3.97	46JOH/PRO2 65FIN/MES	(1×C-(H (1×C _d -(l	(1) ₃ (C)) + (1 × H)(C)) + (2 × hexene rsc)	C-(H)2(C)(C	C _d)) + (2 × C-(1	(tertiary))+
$\Delta_t G^\circ = \ln K_t =$ Liquid Pha	- 263.09	-24.15 -260.28			(1×C-(H (1×C _d -(l	(1) ₃ (C)) + (1 × H)(C)) + (2 × hexene rsc)	C-(H) ₂ (C)(C	C _d)) + (2 × C-(1	(tertiary)) + H) ₂ (C) ₂) +
$\Delta_t G^\circ = \ln K_t = $ Liquid Pha $\Delta_t H^\circ = $ $C_p^\circ = $	263.09 271.04	-24.15 -260.28 275.01	-3.97	65FIN/MES	(1×C-(H (1×C _d -(l	(1) ₃ (C)) + (1 × H)(C)) + (2 × hexene rsc)	C-(H) ₂ (C)(C	C _d)) + (2 × C-(1	(tertiary)) + H) ₂ (C) ₂) +
$\Delta_t G^\circ = \ln K_t = 1$ Liquid Pha $\Delta_t H^\circ = C_p^\circ = S^\circ = 1$	263.09 271.04	-24.15 -260.28 275.01 343.55	-3.97	65FIN/MES	(1×C-(H (1×C _d -(l	(1) ₃ (C)) + (1 × H)(C)) + (2 × hexene rsc)	C-(H) ₂ (C)(C	C _d)) + (2 × C-(1	(tertiary)) + H) ₂ (C) ₂) +
$\Delta_t G^\circ = \ln K_t = \frac{1}{\ln K_t}$ Liquid Pha $\Delta_t H^\circ = \frac{C_p^\circ = S^\circ = \Delta_t S^\circ = \frac{1}{\ln K_t}}{\Delta_t S^\circ = \frac{1}{\ln K_t}}$	263.09 271.04	-24.15 -260.28 275.01 343.55 -1019.56	-3.97	65FIN/MES	(1 × C-(H (1 × C _d -(l (1 × Cyclo	(1) ₃ (C)) + (1 × H)(C)) + (2 × hexene rsc)	C-(H) ₂ (C)(C	C _d)) + (2 × C-(1	(tertiary)) + H) ₂ (C) ₂) +
$\Delta_t G^\circ = \ln K_t = 1$ Liquid Pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = 1$	263.09 271.04	-24.15 -260.28 275.01 343.55 -1019.56 43.70	-3.97	65FIN/MES	(1 × C-(H (1 × C _d -(l (1 × Cyclo	(1) ₃ (C))+(1> H)(C))+(2> phexene rsc) Literature	C-(H) ₂ (C)(C - Calculated	= Residual	(tertiary)) + H) ₂ (C) ₂) + Reference
$\Delta_{\rm f}G^{\circ} = \ln K_{\rm f} = 1$ Liquid Pha $\Delta_{\rm f}H^{\circ} = C_{\rm p}^{\circ} = S^{\circ} = \Delta_{\rm f}S^{\circ} = 1$ $\Delta_{\rm f}G^{\circ} = 1$ $\ln K_{\rm f} = 1$	263.09 271.04 344.97	-24.15 -260.28 275.01 343.55 -1019.56 43.70	-3.97	65FIN/MES 65FIN/MES	$(1 \times C - (H + C)))))))))))))$ Gas Phase $\Delta_{\ell}H^{o} = C_{\rho}^{o} =$	(l) ₃ (C)) + (1 > H)(C)) + (2 > Shexene rsc) Literature -43.26	C-(H) ₂ (C)(C - Calculated -41.47	= Residual	(tertiary)) + H) ₂ (C) ₂) + Reference
$\Delta_{\rm f}G^{\circ} = \ln K_{\rm f} = 1$ Liquid Pha $\Delta_{\rm f}H^{\circ} = C_{\rm f}^{\circ} = S^{\circ} = \Delta_{\rm f}S^{\circ} = 1$ $\Delta_{\rm f}G^{\circ} = 1$ Pentylcyclo	— 263.09 271.04 344.97	-24.15 -260.28 275.01 343.55 -1019.56 43.70 -17.63	-3.97 1.42	65FIN/MES 65FIN/MES C ₁₁ H ₂₂	$(1 \times C - (H + C)))))))))))))$ Gas Phase $\Delta_t H^o = \{ A_t A_t A_t A_t A_t A_t A_t A_t A_t A_t$	(l) ₃ (C)) + (1 > H)(C)) + (2 > Shexene rsc) Literature -43.26	C-(H) ₂ (C)(C - Calculated -41.47	= Residual	(tertiary)) + H) ₂ (C) ₂) + Reference
$\Delta_{\rm f}G^{\circ}= \ln K_{\rm f}= $ $\ln K_{\rm f}= $ Liquid Pha $\Delta_{\rm f}H^{\circ}= C_{\rm f}^{\circ}= S^{\circ}= $ $\Delta_{\rm f}S^{\circ}= \Delta_{\rm f}G^{\circ}= $ $\ln K_{\rm f}= $ Pentylcyclo $(1\times C-(1\times C))$	263.09 271.04 344.97 оhехане H) ₃ (C)) + (1	-24.15 -260.28 275.01 343.55 -1019.56 43.70	-3.97 1.42 + (9 × C−(H) ₂ (65FIN/MES 65FIN/MES C ₁₁ H ₂₂	$(1 \times C - (H + C + C) + C)$ $(1 \times C) + C$ $(1 \times C - (H + C) + C)$ $(1 \times C - (H + C) + C)$ $(2 \times C - (H + C) + C)$ $(3 \times C - (H + C) + C)$ $(4 \times C - (H + C) + C)$ $(5 \times C - (H + C) + C)$ $(6 \times C - (H + C) + C)$ $(7 \times C - (H + C) + C)$ $(8 \times C - (H + C) + C)$ $(9 \times C - (H + C) + C)$ $(9 \times C - (H + C) + C)$ $(9 \times C - (H + C) + C)$ $(1 \times C) + C$ $(1 \times C$	(l) ₃ (C)) + (1 > (1) ₄ (C)) + (2 > (2 > (2 + (2 + (2 + (2 + (2 + (2	C-(H) ₂ (C)(C - Calculated -41.47 127.11	= Residual - 1.79	(tertiary)) + H) ₂ (C) ₂) + Reference 60CAM/ROS
$\Delta_{\rm f}G^{\circ}= \ln K_{\rm f}= $ $\ln K_{\rm f}= $ Liquid Pha $\Delta_{\rm f}H^{\circ}= C_{\rm f}^{\circ}= S^{\circ}= $ $\Delta_{\rm f}S^{\circ}= \Delta_{\rm f}G^{\circ}= $ $\ln K_{\rm f}= $ Pentylcyclo $(1\times C-(1\times C))$	263.09 271.04 344.97 оheхане H) ₃ (C)) + (1	-24.15 -260.28 275.01 343.55 -1019.56 43.70 -17.63 × C-(H)(C) ₃)-	-3.97 1.42 + (9 × C−(H) ₂ (65FIN/MES 65FIN/MES C ₁₁ H ₂₂	$(1 \times C - (H + C + C) + C + C)$ $(1 \times C) + C + C$ $(1 \times C) + C + C$ $(1 \times C) + C + C$ $C + C $	(l) ₃ (C)) + (1 > (1) ₄ (C)) + (2 > (2 > (2 + (2 + (2 + (2 + (2 + (2	-41.47 127.11 -80.46	= Residual - 1.79	(tertiary)) + H) ₂ (C) ₂) + Reference 60CAM/ROS
$\Delta_{\rm f}G^{\circ}= \ln K_{\rm f}= $ $\ln K_{\rm f}= $ Liquid Pha $\Delta_{\rm f}H^{\circ}= C_{\rm f}^{\circ}= S^{\circ}= $ $\Delta_{\rm f}S^{\circ}= \Delta_{\rm f}G^{\circ}= $ $\ln K_{\rm f}= $ Pentylcyclo $(1\times C-(1\times C))$	263.09 271.04 344.97 •• Shexane H) ₃ (C)) + (1 •• Shexane (su	-24.15 -260.28 275.01 343.55 -1019.56 43.70 -17.63 × C-(H)(C) ₃)-	-3.97 1.42 + (9 × C−(H) ₂ (c)	65FIN/MES 65FIN/MES C ₁₁ H ₂₂	$(1 \times C - (H + C + C) + C + C)$ $(1 \times C) + C + C + C$ $(1 \times C) + C + C + C + C$ $(1 \times C) + C + C + C + C$ $(1 \times C - (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times C - (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) + C$ $(1 \times (H + C) + C) $	(l) ₃ (C)) + (1 > (1) ₄ (C)) + (2 > (2 > (2 + (2 + (2 + (2 + (2 + (2	-41.47 127.11 -80.46 183.46	= Residual - 1.79	(tertiary)) + H) ₂ (C) ₂) + Reference 60CAM/ROS
$\Delta_{\rm f}G^{\circ}= { m ln}K_{\rm f}= { m ln}K_{\rm f}= { m ln}K_{\rm f}= { m ln}K_{\rm f}= { m c}_{\rm f}G^{\circ}= { m ln}K_{\rm f}= { m ln}K_{\rm$	263.09 271.04 344.97 •• Shexane H) ₃ (C)) + (1 •• Shexane (su	-24.15 -260.28 275.01 343.55 -1019.56 43.70 -17.63 × C-(H)(C) ₃)- bb) rsc), σ = 3	-3.97 1.42 + (9 × C−(H) ₂ (c)	65FIN/MES 65FIN/MES C ₁₁ H ₂₂ C) ₂) +	$(1 \times C - (H + C + C) + C + C)$ $(1 \times C) + C + C + C$ $(1 \times C) + C + C + C + C$ $(1 \times C) + C + C + C$ $(1 \times C - (H + C) + C)$ $(1 \times C - (H + C) + C)$ $(1 \times C - (H + C) + C)$ $(2 \times C) + C + C$ $(3 \times C - (H + C) + C)$ $(4 \times C - (H + C) + C)$ $(5 \times C) + C + C$ $(6 \times C) + C + C$ $(7 \times C - (H + C) + C)$ $(1 \times C - (H + C) + C)$ $(1 \times C - (H + C) + C)$ $(2 \times C) + C$ $(3 \times C) + C$ $(4 \times C) + C$ $(5 \times C) + C$ $(6 \times C) + C$ $(7 \times C) + C$ $(8 \times C) + C$ $(9 \times C) + C$ $(1 \times C) + C$ $(1$	(l) ₃ (C)) + (1 > (1) ₄ (C)) + (2 > (2 > (2 + (2 + (2 + (2 + (2 + (2	-41.47 127.11 -80.46 183.46 239.49	= Residual - 1.79	(tertiary)) + H) ₂ (C) ₂) + Reference 60CAM/ROS
$\Delta_{t}G^{\circ} = \ln K_{t} = 1$ Liquid Pha $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = 1$ Pentylcyclo $(1 \times C - (1 \times C))$	263.09 271.04 344.97 Shexane H) ₃ (C)) + (1 Ohexane (su	-24.15 -260.28 275.01 343.55 -1019.56 43.70 -17.63 × C-(H)(C) ₃)- bb) rsc), σ = 3	-3.97 1.42 + (9 × C−(H) ₂ (c)	65FIN/MES 65FIN/MES C ₁₁ H ₂₂ C) ₂) +	$(1 \times C - (H + C + C) - (H + C) - ($	(l) ₃ (C)) + (1 > (1) ₄ (C)) + (2 > (2 > (2 + (2 + (2 + (2 + (2 + (2	-41.47 127.11 -80.46 183.46 239.49 -584.12	= Residual - 1.79	(tertiary)) + H) ₂ (C) ₂) + Reference 60CAM/ROS
$\Delta_{t}G^{\circ} = \ln K_{t} = 1$ Liquid Pha $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = 1$ Pentylcyclo $(1 \times C - (1 \times C))$ Gas Phase	263.09 271.04 344.97 Shexane H) ₃ (C)) + (1 Ohexane (su	-24.15 -260.28 275.01 343.55 -1019.56 43.70 -17.63 × C-(H)(C) ₃)- bb) rsc), σ = 3	-3.97 1.42 + (9 × C−(H) ₂ (c)	65FIN/MES 65FIN/MES C ₁₁ H ₂₂ C) ₂) +	$(1 \times C - (H + C))))))))))))$ Liquid Phase $\Delta_{I}H^{\circ} = C^{\circ}_{\rho} = C^{\circ}_{\rho} = \Delta_{I}S^{\circ} = \Delta_{I}G^{\circ} = \Delta_{I}G^{\circ} = \Delta_{I}G^{\circ}$	(l) ₃ (C)) + (1 > (1) ₄ (C)) + (2 > (2 > (2 + (2 + (2 + (2 + (2 + (2	-41.47 127.11 -80.46 183.46 239.49 -584.12 93.69	= Residual - 1.79	(tertiary)) + H) ₂ (C) ₂) + Reference 60CAM/ROS
$\Delta_{t}G^{\circ} = \ln K_{t} = 1$ Liquid Pha $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = 1$ Pentylcyclo $(1 \times C - (1 \times C) + C_{t})$ Gas Phase $\Delta_{t}H^{\circ} = 1$	263.09 271.04 344.97 Shexane H) ₃ (C)) + (1 Ohexane (su	-24.15 -260.28 275.01 343.55 -1019.56 43.70 -17.63 × C-(H)(C) ₃)- bb) rsc), σ = 3	-3.97 1.42 + (9 × C−(H) ₂ (c)	65FIN/MES 65FIN/MES C ₁₁ H ₂₂ C) ₂) +	$(1 \times C - (H + C))))))))))))$ Liquid Phase $\Delta_{I}H^{\circ} = C^{\circ}_{I} = C^{\circ}_{I} = \Delta_{I}S^{\circ} = \Delta_{I}S^{\circ} = \Delta_{I}G^{\circ} = \Delta_{I}G^{\circ}$	(l) ₃ (C)) + (1 > (1) ₄ (C)) + (2 > (2 > (2 + (2 + (2 + (2 + (2 + (2	-41.47 127.11 -80.46 183.46 239.49 -584.12 93.69	= Residual - 1.79	(tertiary)) + H) ₂ (C) ₂) + Reference 60CAM/ROS
$\Delta_{l}G^{\circ} = \ln K_{l} = 1$ Liquid Pha $\Delta_{l}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{l}S^{\circ} = \ln K_{l} = 1$ Pentylcyclo $(1 \times C - (1 \times C) + C)$ Gas Phase $\Delta_{l}H^{\circ} = C_{p}^{\circ} = C_{p}^{\circ} = 1$	263.09 271.04 344.97 Shexane H) ₃ (C)) + (1 Ohexane (su	-24.15 -260.28 275.01 343.55 -1019.56 43.70 -17.63 × C-(H)(C) ₃)-1b) rsc), σ = 3 re - Calculated	-3.97 1.42 + (9 × C−(H) ₂ (c)	65FIN/MES 65FIN/MES C ₁₁ H ₂₂ C) ₂) +	$(1 \times C - (H + C))))))))))))$ Liquid Phase $\Delta_{I}H^{\circ} = C^{\circ}_{I} = C^{\circ}_{I} = \Delta_{I}S^{\circ} = \Delta_{I}S^{\circ} = \Delta_{I}G^{\circ} = \Delta_{I}G^{\circ}$	(l) ₃ (C)) + (1 > (1) ₄ (C)) + (2 > (2 > (2 + (2 + (2 + (2 + (2 + (2	-41.47 127.11 -80.46 183.46 239.49 -584.12 93.69	= Residual - 1.79	(tertiary)) + H) ₂ (C) ₂) + Reference 60CAM/ROS
$\Delta_l G^\circ = \ln K_f = \frac{1}{2}$ Liquid Pha $\Delta_l H^\circ = \frac{1}{2}$ $S^\circ = \frac{1}{2}$ $\Delta_l S^\circ = \frac{1}{2}$ $\Delta_l G^\circ = \frac{1}{2}$ $\Delta_l G^\circ = \frac{1}{2}$ $\Delta_l G^\circ = \frac{1}{2}$ Gas Phase $\Delta_l H^\circ = \frac{1}{2}$ $C_l^\circ = \frac{1}{2}$ $C_l^\circ = \frac{1}{2}$ $C_l^\circ = \frac{1}{2}$	263.09 271.04 344.97 Shexane H) ₃ (C)) + (1 Ohexane (su	- 24.15 - 260.28 275.01 343.55 - 1019.56 43.70 - 17.63 × C-(H)(C) ₃)- ib) rsc), σ = 3 re - Calculated - 229.49 229.00 501.00	-3.97 1.42 + (9 × C-(H) ₂ (1) = Residual	65FIN/MES 65FIN/MES C ₁₁ H ₂₂ C) ₂)+	$(1 \times C - (H + C))))))))))))$ Liquid Phase $\Delta_{I}H^{\circ} = C^{\circ}_{I} = C^{\circ}_{I} = \Delta_{I}S^{\circ} = \Delta_{I}S^{\circ} = \Delta_{I}G^{\circ} = \Delta_{I}G^{\circ}$	(l) ₃ (C)) + (1 > (1) ₄ (C)) + (2 > (2 > (2 + (2 + (2 + (2 + (2 + (2	-41.47 127.11 -80.46 183.46 239.49 -584.12 93.69	= Residual - 1.79	(tertiary)) + H) ₂ (C) ₂) + Reference 60CAM/ROS
$\Delta_{l}G^{\circ} = \ln K_{l} = 1$ Liquid Pha $\Delta_{l}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{l}S^{\circ} = 1$ $\ln K_{l} = 1$ Pentylcyclo $(1 \times C - (1 \times C) + C)$ Gas Phase $\Delta_{l}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{l}S^{\circ} = 1$	-263.09 271.04 344.97 Shexane H) ₃ (C))+(1 lohexane (su Literatur	- 24.15 - 260.28 275.01 343.55 - 1019.56 43.70 - 17.63 × C-(H)(C) ₃) - ab) rsc), σ = 3 re - Calculated - 229.49 229.00	-3.97 1.42 + (9 × C-(H) ₂ (1) = Residual	65FIN/MES 65FIN/MES C ₁₁ H ₂₂ C) ₂) + Reference	$(1 \times C - (H + C))))))))))))$ Liquid Phase $\Delta_{I}H^{\circ} = C^{\circ}_{I} = C^{\circ}_{I} = \Delta_{I}S^{\circ} = \Delta_{I}S^{\circ} = \Delta_{I}G^{\circ} = \Delta_{I}G^{\circ}$	(l) ₃ (C)) + (1 > (1) ₄ (C)) + (2 > (2 > (2 + (2 + (2 + (2 + (2 + (2	-41.47 127.11 -80.46 183.46 239.49 -584.12 93.69	= Residual - 1.79	(tertiary)) + H) ₂ (C) ₂) + Reference 60CAM/ROS
$\Delta_{l}G^{\circ} = \ln K_{l} = 1$ Liquid Pha $\Delta_{l}H^{\circ} = C_{l}^{\circ} = S^{\circ} = \Delta_{l}S^{\circ} = \ln K_{l} = 1$ Pentylcyclo $(1 \times C - (1 \times C) + C)$ Gas Phase $\Delta_{l}H^{\circ} = C_{l}^{\circ} = S^{\circ} = S^{\circ} = S^{\circ} = S^{\circ} = 1$	-263.09 271.04 344.97 Shexane H) ₃ (C))+(1 lohexane (su Literatur	- 24.15 - 260.28 275.01 343.55 - 1019.56 43.70 - 17.63 × C-(H)(C) ₃)- ib) rsc), σ = 3 re - Calculated - 229.49 229.00 501.00	-3.97 1.42 + (9 × C-(H) ₂ (1) = Residual	65FIN/MES 65FIN/MES C ₁₁ H ₂₂ C) ₂) + Reference	$(1 \times C - (H + C))))))))))))$ Liquid Phase $\Delta_{I}H^{\circ} = C^{\circ}_{I} = C^{\circ}_{I} = \Delta_{I}S^{\circ} = \Delta_{I}S^{\circ} = \Delta_{I}G^{\circ} = \Delta_{I}G^{\circ}$	(l) ₃ (C)) + (1 > (1) ₄ (C)) + (2 > (2 > (2 + (2 + (2 + (2 + (2 + (2	-41.47 127.11 -80.46 183.46 239.49 -584.12 93.69	= Residual - 1.79	(tertiary)) + H) ₂ (C) ₂) + Reference 60CAM/ROS

1-Ethylcyclo (1×C-(H (1×C _d -(I	ohexene (I) ₃ (C)) + (3 × C-(H)(C)) + (2 × C-(H)2(C)(C, H)2(C)2) -	ı))+(1×C _d -(+(1×Cyclohe	C_8H_{14} $C)_2) +$ xene rsc)		cosane C)) + $(2 \times C - (H)(C)_3)$ + xane (sub) rsc)	(22×C-(H) ₂	C ₂₆ H ₅₂ ((C) ₂)+
	Literature – Ca	alculated =	= Residual	Reference		iterature – Calculated =	= Residual	Reference
Gas Phase $\Delta_{\epsilon}H^{\circ} = C_{p}^{\circ} =$		60.09 47.74	-3.34	60CAM/ROS	Gas Phase $\Delta_t H^\circ = C_\rho^\circ =$	-541.11 572.38		
Liquid Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = 1$ $\Delta_t G^\circ = 1$ $\ln K_t = 1$	-106.69 -1 2 2 -6	04.01 12.75 71.16 88.76 01.34 40.88	-2.68	61LAB/ROS	Liquid Phase $\Delta_t H^\circ = -60$ $C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = -60$	66.09 -672.88 758.75 856.28 -2687.81 128.49 -51.83	6.79	44KNO/HUF
	exane H) ₂) + (1 × C _d (H H)(C) ₃) + (5 × C(cosane (C)) + (2 × C-(H)(C) ₃) + (xane (sub) rsc)	(22×C-(H) ₂	C ₂₆ H ₅₂ (C) ₂)+
	Literature – C	alculated =	= Residual	Reference	L	iterature – Calculated =	= Residual	Reference
Gas Phase $\Delta_i H^o = C_p^o =$		62.95 72.46			Gas Phase $\Delta_t H^\circ = C_p^\circ =$	- 541.11 572.38		·
Liquid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	233.47 - 1	.08.41 229.53 309.55 786.68 126.14 50.88	3.94	79FUC/PEA	Liquid Phase $\Delta_{t}H^{\circ} = -6^{\circ}$ $C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = 0$	74.04 - 672.88 758.75 856.28 - 2687.81 128.49 - 51.83	- 1.16	44KNO/HUF
(1 × C-(I (2 × C-(I	cyclohexane H) ₃ (C)) + $(1 \times C_{d}$ H) ₂ (C)(C _d)) + $(3 \times C_{d})$ ohexane (sub) rs	(C-(H) ₂ (C ₈ H ₁₄ +	11-Cyclohexylho (2×C-(H) ₃ ((1×Cyclohex	eneicosane C))+(2×C-(H)(C) ₃)+ kane (sub) rsc)	(23×C-(H) ₂	C ₂₇ H ₅₄ (C) ₂)+
(2110)0	Literature – C		= Residual	Reference	L	iterature – Calculated =	= Residual	Reference
Gas Phase $\Delta_t H^\circ = C_p^\circ =$		65.84 146.68			Gas Phase $\Delta_l H^\circ = C_p^\circ =$	-561.74 595.27		
Liquid Pha $ \Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	203.76	108.11 207.93 267.63 592.29 98.30 39.65	-4.17	79FUC/PEA	Liquid Phase $\Delta_t H^\circ = -6t$ $C_\rho^\circ = \\ S^\circ = \\ \Delta_t S^\circ = \\ \Delta_t G^\circ = \\ \ln K_t = $	89.94 - 698.61 789.17 888.66 - 2791.74 133.75 - 53.95	8.67	44KNO/HUF

TABLE 13. Cyclic CH-02 (48) - Continued

	$_{3}(C))+(2$	\times C-(H)(C) ₃)+(27×C-(H) ₂	$C_{31}H_{62}$ (C) ₂)+	cis-Decalin (2×C-(H	H)(C) ₃)+(8	\times C-(H) ₂ (C) ₂) -	+ (1 × cis - Dec	C _{ie} H _i alin rsc)
(1 × Cyclo	hexane (su Literatur	e – Calculated =	Residual	Reference		Literatu	re – Calculated =	= Residual	Reference
					Gas Phase				
Gas Phase					$\Delta_t H^\circ =$	-40.38	-40.38	0.00	69STU/WES
$\Delta_t H^\circ =$	'	-644.26			$C_p^{\circ} =$	39.84	39.84	0.00	69STU/WES
$C_p^{\circ} =$		686.83							
				-	Liquid Phas	se			
Liquid Phas				47	-	- 219.40	-219.40	0.00	60SPE/ROS
$\Delta_{\mathbf{f}}H^{\circ} =$	- 792.45	-801.53	9.08	46PAR/WES	$C_p^{\circ} =$	232.00	232.00	0.00	57MCC/FIN
$C_p^{\circ} =$		910.85			S° =	265.01	265.01	0.00	57MCC/FIN
S° =		1018.18			$\Delta_{\mathfrak{p}} S^{\circ} =$		- 967.53		
$\Delta_f S^\circ =$		-3207.46			$\Delta_t G^{\circ} =$		69.07		
$\Delta_f G^\circ = \ln K_f =$		154.77 62.43			$lnK_f =$		- 27.86		
is-Hexahyd	Iroindan			C ₉ H ₁₆	trans-Decal		×C-(H) ₂ (C) ₂) -	+ (1 × trans -D	C ₁₆ H
(2×C-(H		\times C-(H) ₂ (C) ₂) +					re – Calculated =		Reference
(1 ~ 65 - 1)	•	·	.	Defense				- Residual	
	Literatu	re – Calculated =	Residual	Reference	Gas Phase				
					$\Delta_t H^\circ =$	-43.57	-43.57	0.00	69STU/WES
Gas Phase					$C_p^{\circ} =$	40.04	40.04	0.00	69STU/WES
$\Delta_t H^{\circ} =$	- 127.24	- 127.24	0.00	60BRO/ROS					
		11 L. L. 21 W. M.			Liquid Phas				
Liquid Pha						- 230.60	-230.60	0.00	60SPE/ROS
$\Delta_t H^\circ =$	- 173.26	- 173.26	0.00	60BRO/ROS	$C_p^{\circ} =$	228.49	228.49	0.00	57MCC/FIN
$C_p^{\circ} =$	214.18	214.18	0.00	72FIN/MCC	S° =	264.93	264.93	0.00	57MCC/FIN
S° =	265.47	265.47	0.00	72FIN/MCC	$\Delta_f S^\circ =$		- 967.61		
$\Delta_f S^\circ =$		- 830.76			$\Delta_f G^\circ =$		57.89		
$\Delta_{\rm f}G^{\circ} =$		74.43			$lnK_f =$		-23.35		
$lnK_t =$		-30.02				·			
					Bicyclo[2.2.	2}octane			C₄H₁
trans-Hexal	hydroindan	ı		C ₂ H ₁₆			\times C-(H) ₂ (C) ₂) +	+	
(2×C-(H	$-1)(C)_3) + (7)_4$	$7 \times C - (H)_2(C)_2 + (H)_2(C)_2$			(1×Bicyo	clo[2.2.2]oc	tane rsc)		
(1×trans	-Hexahydr	oindan rsc)							
	Literatu	re – Calculated =	Residual	Reference		Literatu	re – Calculated =	= Residual	Reference
					Gas Phase				
Gas Phase					$\Delta_{\rm f} H^{\circ} =$	-99.00	- 99.00	0.00	71WON/WES
$\Delta_t H^\circ =$	-131.59	131.59	0.00	60BRO/ROS					
					Liquid Phas	se			
Liquid Pha					$C_p^{\circ} =$		157.69		
$\Delta_t H^{\circ} -$	-176.36	176.36	0.00	60BRO/ROS	S° =		83.05		
$C_p^{\circ} =$	209.70	209.70	0.00	72FIN/MCC	$\Delta_f S^\circ =$		 876.87		
	258.86	258.86	0.00	72FIN/MCC					
S° =		000.00							
$S^{\circ} = \Delta_{f}S^{\circ} =$		- 837.37							
S° =		- 837.37 73.30			Solid Phase Δ _t H° =			0.00	71WON/WES

(4 × C-(H))(C) ₃)+(6)				$(1 \times 2, 2 - Pa$	nacyclopiid			
	Literatur	e – Calculated =	Residual	Reference		Literatur	e – Calculated =	= Residual	Reference
Gas Phase						- No			
$\Delta_{\rm f} H^{\circ} = -$	- 134.60 	- 134.60	0.00	70MAN/RAP	Gas Phase $\Delta_f H^\circ =$	244.70	244.77	-0.07	80NIS/SAK
Solid Phase Δ _t H° = -	- 197.20	- 197.20	0.00	70MAN/RAP	Solid Phase				
		<u> </u>			$\Delta_f H^\circ = C_p^\circ =$	146.70 252.34	146.70 252.34	0.00 0.00	80NIS/SAK 70AND/WES
					S° =	265.68	265.68	0.00	70AND/WES
Bicyclo[3.3.3	lundecane			$C_{11}H_{20}$	$\Delta_f S^\circ =$		-870.73	5.55	, 0, 11, 12, 11, 125,
		\times C-(H) ₂ (C) ₂) +	-		$\Delta_f G^\circ =$		406.31		
		decane rsc)			$lnK_f =$		- 163.90		
	Literatur	e – Calculated =	= Residual	Reference					
Gas Phase					3,3-Paracycle (8×C _B -(F		$(4 \times C_B - (C)(C_B))$) ₂) + (4 × C-(1	$C_{18}H_{2}$ H) ₂ (C)(C _B))+
$\Delta_f H^\circ =$	- 88.95	-88.95	0.00	75PAR/STE			×3,3-Paracyclo)-\
Solid Phase						Literatur	e – Calculated =	= Residual	Reference
	- 152.55	-152.55	0.00	75PAR/STE					
					Gas Phase				
					$\Delta_f H^o =$	129.37	129.37	0.00	69SHI/MCN
				0.77	$\Delta_f H^\circ =$	129.37	129.37	0.00	69SHI/MCN
		(4 × C ₂ (C)(C ₂)	h)+(4×C-(1	C ₁₆ H ₁₆ H) ₂ (C)(C _B)) +		129.37	129.37	0.00	69SHI/MCN
(8×C _B −(I	$H)(C_B)_2) +$	(4×C _B –(C)(C _B)			$\Delta_t H^\circ =$ Solid Phase $\Delta_t H^\circ =$	129.37 26.15	26.15	0.00	69SHI/MCN
$(8 \times C_B - (1$	$H)(C_B)_2) + COTT) + (1 > COTT)$	2,2-Metacyclop	hane rsc)	$H_{2}(C)(C_{B})$ +	Solid Phase			***************************************	
(8×C _B −(I	$H)(C_B)_2) + COTT) + (1 > COTT)$		hane rsc)		Solid Phase $\Delta_t H^\circ =$	26.15	26.15	0.00	69SHI/MCN
	H)(C _B) ₂) + corr) + (1 > Literatur	2,2-Metacyclop	ohane rsc) = Residual	H) ₂ (C)(C _B))+ Reference	Solid Phase $\Delta_t H^\circ = C_\rho^\circ =$ Indane	26.15 324.26	26.15 324.26	0.00 0.00	69SHI/MCN 69SHI/MCN C ₂ H ₁
(8×C _B -(I	$H)(C_B)_2) + COTT) + (1 > COTT)$	2,2-Metacyclop	hane rsc)	$H_{2}(C)(C_{B})$ +	Solid Phase $\Delta_t H^\circ = C_p^\circ =$ Indane $(4 \times C_B - (1 + C_B))$	26.15 324.26 H)(C _B) ₂)+(26.15 324.26	0.00 0.00 C _B) ₂) + (2 × C	69SHI/MCN 69SHI/MCN C ₂ H ₁ C-(H) ₂ (C)(C _D)) +
(8 × C _B -(I (2 × meta	H)(C _B) ₂) + (1 × corr) + (1 × Literatus	2,2-Metacyclop	ohane rsc) = Residual	H) ₂ (C)(C _B))+ Reference	Solid Phase $\Delta_t H^\circ = C_p^\circ =$ Indane $(4 \times C_B - (1 + C_B))$	26.15 324.26 F)(C _B) ₂) + (1) ₂ (C) ₂) + (1	26.15 324.26 2×C _{BF} -(C _{BF})(0.00 0.00 C _D) ₂) + (2 × C e rsc (unsub)	69SHI/MCN 69SHI/MCN C ₂ H ₁ C-(H) ₂ (C)(C _D)) +
$(8 \times C_8 - (1 \times C_8 - (1 \times C_8 + (2 \times meta))))$ Gas Phase $\Delta_t H^\circ =$ Solid Phase $\Delta_t H^\circ =$	H)(C _B) ₂) + corr) + (1 > Literatur 170.50	2,2-Metacyclor re — Calculated = 170.50 78.50	hane rsc) = Residual 0.00	H) ₂ (C)(C _B)) + Reference 69SHI/MCN	Solid Phase $\Delta_t H^\circ = C_p^\circ =$ Indane $(4 \times C_B - (1 + C_B))$	26.15 324.26 F)(C _B) ₂) + (1) ₂ (C) ₂) + (1	26.15 324.26 2×C _{BF} -(C _{BF})(× Cyclopenten	0.00 0.00 C _D) ₂) + (2 × C e rsc (unsub)	69SHI/MCN 69SHI/MCN C ₅ H ₁ C-(H) ₂ (C)(C _D)) +
$(8 \times C_8 - (1 \times C_8 - (1 \times C_8 + (2 \times meta))))$ Gas Phase $\Delta_t H^{\circ} =$ Solid Phase	H)(C _B) ₂) + (1 × corr) + (1 × Literatus	2,2-Metacyclop re – Calculated = 170.50	hane rsc) = Residual 0 00	H) ₂ (C)(C _B)) + Reference 69SHI/MCN	Solid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Indane $(4 \times C_{B} - (H_{\ell})^{\circ})$ $(1 \times C - (H_{\ell})^{\circ})$	26.15 324.26 F)(C _B) ₂) + (1) ₂ (C) ₂) + (1	26.15 324.26 2×C _{BF} -(C _{BF})(× Cyclopenten	0.00 0.00 C _D) ₂) + (2 × C e rsc (unsub)	69SHI/MCN 69SHI/MCN C ₅ H ₁ C-(H) ₂ (C)(C _D)) +
$(8 \times C_8 - (1 \times C_8 - (1 \times C_8 + (2 \times meta))))$ Gas Phase $\Delta_t H^\circ =$ Solid Phase $\Delta_t H^\circ =$	H)(C _B) ₂) + corr) + (1 > Literatur 170.50	2,2-Metacyclor re — Calculated = 170.50 78.50	hane rsc) = Residual 0.00	H) ₂ (C)(C _B)) + Reference 69SHI/MCN	Solid Phase $\Delta_t H^o = C_p^o =$ Indane $(4 \times C_B - (+ (1 \times C - (H))))$ Gas Phase	26.15 324.26 $H(C_B)_2 + (D_2(C)_2) + (D_2($	26.15 324.26 2×C _{BF} -(C _{BF})(× Cyclopentence – Calculated =	0.00 0.00 C _B) ₂) + (2 × C e rsc (unsub) = Residual	69SHI/MCN 69SHI/MCN C ₃ H ₁ C-(H) ₂ (C)(C _D)) +) Reference
$(8 \times C_8 - (1 \times C_8 - (1 \times C_8 + (2 \times meta))))$ Gas Phase $\Delta_t H^\circ =$ Solid Phase $\Delta_t H^\circ =$	H)(C _B) ₂) + corr) + (1 > Literatur 170.50	2,2-Metacyclor re — Calculated = 170.50 78.50	hane rsc) = Residual 0.00	H) ₂ (C)(C _B)) + Reference 69SHI/MCN 69SHI/MCN 69SCH/MCN	Solid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Indane $(4 \times C_{B} - (H_{\ell})^{\circ})$ $(1 \times C - (H_{\ell})^{\circ})$	26.15 324.26 F)(C _B) ₂) + (1) ₂ (C) ₂) + (1	26.15 324.26 2×C _{BF} -(C _{BF})(× Cyclopenten	0.00 0.00 C _D) ₂) + (2 × C e rsc (unsub)	69SHI/MCN 69SHI/MCN C ₅ H ₁ C-(H) ₂ (C)(C _D)) +
$(8 \times C_{B}-(1 \times C_{B}-(1 \times C_{B}))^{2})$ Gas Phase $\Delta_{t}H^{o} = $ Solid Phase $\Delta_{t}H^{o} = $ $C_{p}^{o} = $ 2,2-Metapar	H)(C _B) ₂) + corr) + (1 > Literatus 170.50 78.50 240.60	78.50 240.60	0.00 0.00 0.00	H) ₂ (C)(C _B)) + Reference 69SHI/MCN 69SHI/MCN 69SCH/MCN C ₁₆ H ₁₆	Solid Phase $\Delta_t H^\circ = C_p^\circ =$ Indane $(4 \times C_B - (+ (1 \times C - (H))))$ Gas Phase $\Delta_t H^\circ =$	26.15 324.26 $H(C_B)_2 + (D_2(C)_2) + (D_2($	26.15 324.26 $2 \times C_{BF} - (C_{BF})($ $\times \text{Cyclopentene}$ $e - \text{Calculated} =$ 56.31	0.00 0.00 C _B) ₂) + (2 × C e rsc (unsub) = Residual	69SHI/MCN 69SHI/MCN C ₉ H ₁ C-(H) ₂ (C)(C _D)) +) Reference
$(8 \times C_8-(I + C_8-(I + C_8) + C_8-(I + C_8))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = C$	H)(C _B) ₂) + corr) + (1 > Literatur 170.50 78.50 240.60 racyclophar H)(C _B) ₂) +	78.50 240.60	0.00 0.00 0.00 0.00	H) ₂ (C)(C _B)) + Reference 69SHI/MCN 69SHI/MCN 69SCH/MCN C ₁₆ H ₁₆ H) ₂ (C)(C _B)) +	Solid Phase $\Delta_t H^\circ = C_\rho^\circ =$ Indane $(4 \times C_B - (1 \times C (H)))$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ =$	26.15 324.26 H)(C _B) ₂) + (1) ₂ (C) ₂) + (1 Literature 60.90	26.15 324.26 $2 \times C_{BF} - (C_{BF})($ $\times \text{Cyclopentene}$ $e - \text{Calculated} =$ 56.31	0.00 0.00 C _B) ₂) + (2 × C e rsc (unsub) = Residual	69SHI/MCN 69SHI/MCN C ₉ H ₁ C-(H) ₂ (C)(C _D)) +) Reference
$(8 \times C_8-(I + C_8-(I + C_8) + C_8-(I + C_8))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = C$	H)(C _B) ₂) + corr) + (1 > Literatur 170.50 78.50 240.60 racyclophar H)(C _B) ₂) +	78.50 240.60	0.00 0.00 0.00 0.00	H) ₂ (C)(C _B)) + Reference 69SHI/MCN 69SHI/MCN 69SCH/MCN C ₁₆ H ₁₆ H) ₂ (C)(C _B)) +	Solid Phase $\Delta_t H^\circ = C_\rho^\circ =$ Indane $(4 \times C_B - (H + (1 \times C - (H))))$ Gas Phase $\Delta_t H^\circ = C_\rho^\circ =$ Liquid Phase	26.15 324.26 H)(C _B) ₂) + (1) ₂ (C) ₂) + (1 Literature 60.90	26.15 324.26 2.× C _{BF} -(C _{BF})(× Cyclopentender – Calculated =	0.00 0.00 C _B) ₂) + (2 × C e rsc (unsub) = Residual 4.59	69SHI/MCN 69SHI/MCN C ₃ H ₁ C-(H) ₂ (C)(C _D)) +) Reference
$(8 \times C_8-(I + C_8-(I + C_8) + C_8-(I + C_8))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = C$	H)(C _B) ₂)+ corr)+(1> Literatur 170.50 78.50 240.60 racyclophar H)(C _B) ₂)+ corr)+(1>	78.50 240.60	0.00 0.00 0.00 0.00 0.00	H) ₂ (C)(C _B)) + Reference 69SHI/MCN 69SHI/MCN 69SCH/MCN C ₁₆ H ₁₆ H) ₂ (C)(C _B)) +	Solid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Indane $(4 \times C_{B} - (H_{\ell})^{\circ})$ $(1 \times C - (H_{\ell})^{\circ})$ Gas Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Liquid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$	26.15 324.26 H)(C _B) ₂) + (1) ₂ (C) ₂) + (1 Literature 60.90	26.15 324.26 $2 \times C_{BF} - (C_{BF})($ $\times \text{Cyclopentene}$ $e - \text{Calculated} =$ 56.31	0.00 0.00 C _B) ₂) + (2 × C e rsc (unsub) = Residual	69SHI/MCN 69SHI/MCN C ₃ H ₁ C-(H) ₂ (C)(C _D)) +) Reference
$(8 \times C_8-(I + C_8-(I + C_8) + C_8-(I + C_8))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = C$	H)(C _B) ₂)+ corr)+(1> Literatur 170.50 78.50 240.60 racyclophar H)(C _B) ₂)+ corr)+(1>	78.50 240.60 1e – Calculated =	0.00 0.00 0.00 0.00 0.00	H) ₂ (C)(C _B)) + Reference 69SHI/MCN 69SHI/MCN 69SCH/MCN C ₁₆ H ₁₆ H) ₂ (C)(C _B)) +	Solid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Indane $(4 \times C_{B} - (H + (1 \times C - (H))))$ Gas Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Liquid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} =$	26.15 324.26 H)(C _B) ₂) + (1) ₂ (C) ₂) + (1 Literature 60.90	26.15 324.26 22 × C _{BF} – (C _{BF})(× Cyclopentender – Calculated = 56.31 102.02	0.00 0.00 C _B) ₂) + (2 × C e rsc (unsub) = Residual 4.59	69SHI/MCN 69SHI/MCN C ₃ H ₁ C-(H) ₂ (C)(C _D)) +) Reference
$(8 \times C_{B}-(1))$ $(2 \times meta)$ Gas Phase $\Delta_{l}H^{o} =$ $C_{p}^{o} =$ $C_{p}^{o} =$ 2,2-Metapar $(8 \times C_{B}-(1))$ $(1 \times meta)$	H)(C _B) ₂)+ corr)+(1> Literatur 170.50 78.50 240.60 racyclophar H)(C _B) ₂)+ corr)+(1>	78.50 240.60 1e – Calculated =	0.00 0.00 0.00 0.00 0.00	H) ₂ (C)(C _B)) + Reference 69SHI/MCN 69SHI/MCN 69SCH/MCN C ₁₆ H ₁₆ H) ₂ (C)(C _B)) +	Solid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Indane $(4 \times C_{B} - (H))$ $(1 \times C - (H))$ Gas Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Liquid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{\ell}S^{\circ} =$	26.15 324.26 H)(C _B) ₂) + (1) ₂ (C) ₂) + (1 Literature 60.90	26.15 324.26 22 × C _{BI} – (C _{BI})(× Cyclopentente – Calculated = 56.31 102.02 10.40 170.16 279.95 – 424.56	0.00 0.00 C _B) ₂) + (2 × C e rsc (unsub) = Residual 4.59	69SHI/MCN 69SHI/MCN C ₃ H ₁ C-(H) ₂ (C)(C _D)) +) Reference
$(8 \times C_B-(1))^2$ $(2 \times meta)^2$ Gas Phase $\Delta_t H^o =$ Solid Phase $\Delta_t H^o =$ $C_p^o =$ 2,2-Metapar $(8 \times C_B-(1))^2$ $(1 \times meta)^2$ Gas Phase	H)(C _B) ₂) + corr) + (1 > Literatur 170.50 78.50 240.60 racyclophal H)(C _B) ₂) + corr) + (1 > Literatur	78.50 240.60 170.50 78.50 240.60 18e (4 × C _B -(C)(C _B) (2,2-Metaparac)	0.00 0.00 0.00 0.00 0.2) + (4 × C-(1) yclophane rse	H) ₂ (C)(C _B)) + Reference 69SHI/MCN 69SHI/MCN 69SCH/MCN C ₁₆ H ₁₆ H) ₂ (C)(C _B)) + c) Reference	Solid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Indane $(4 \times C_{B} - (\ell + \ell))$ Gas Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Liquid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = \Delta_{\ell}S^{\circ} =$ $\Delta_{\ell}S^{\circ} = \Delta_{\ell}G^{\circ} =$	26.15 324.26 H)(C _B) ₂) + (1) ₂ (C) ₂) + (1 Literature 60.90	26.15 324.26 22 × C _{BI} – (C _{BI})(× Cyclopententer – Calculated = 56.31 102.02 10.40 170.16 279.95 – 424.56 136.98	0.00 0.00 C _B) ₂) + (2 × C e rsc (unsub) = Residual 4.59	69SHI/MCN 69SHI/MCN C ₃ H ₁ C-(H) ₂ (C)(C _D)) +) Reference
$(8 \times C_{B}-(1))$ $(2 \times meta)$ Gas Phase $\Delta_{t}H^{o} =$ Solid Phase $\Delta_{t}H^{o} =$ $C_{p}^{o} =$ 2,2-Metapar $(8 \times C_{B}-(1))$ $(1 \times meta)$	H)(C _B) ₂)+ corr)+(1> Literatur 170.50 78.50 240.60 racyclophar H)(C _B) ₂)+ corr)+(1>	78.50 240.60 1e – Calculated =	0.00 0.00 0.00 0.00 0.00	H) ₂ (C)(C _B)) + Reference 69SHI/MCN 69SHI/MCN 69SCH/MCN C ₁₆ H ₁₆ H) ₂ (C)(C _B)) +	Solid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Indane $(4 \times C_{B} - (H))$ $(1 \times C - (H))$ Gas Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Liquid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{\ell}S^{\circ} =$	26.15 324.26 H)(C _B) ₂) + (1) ₂ (C) ₂) + (1 Literature 60.90	26.15 324.26 22 × C _{BI} – (C _{BI})(× Cyclopentente – Calculated = 56.31 102.02 10.40 170.16 279.95 – 424.56	0.00 0.00 C _B) ₂) + (2 × C e rsc (unsub) = Residual 4.59	69SHI/MCN 69SHI/MCN C ₃ H ₁ C-(H) ₂ (C)(C _D)) +) Reference
$(8 \times C_8 - (1 \times C_8 $	H)(C _B) ₂)+ corr)+(1> Literatur 170.50 78.50 240.60 racyclophar H)(C _B) ₂)+ corr)+(1> Literatur 218.40	78.50 240.60 170.50 78.50 240.60 180.50 240.60 190.50 240.60	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	H) ₂ (C)(C _B)) + Reference 69SHI/MCN 69SHI/MCN 69SCH/MCN C ₁₆ H ₁₆ H) ₂ (C)(C _B)) + c) Reference	Solid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Indane $(4 \times C_{B} - (\ell + \ell))$ Gas Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Liquid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = \Delta_{\ell}S^{\circ} =$ $\Delta_{\ell}S^{\circ} = \Delta_{\ell}G^{\circ} =$	26.15 324.26 H)(C _B) ₂) + (1) ₂ (C) ₂) + (1 Literature 60.90	26.15 324.26 22 × C _{BI} – (C _{BI})(× Cyclopententer – Calculated = 56.31 102.02 10.40 170.16 279.95 – 424.56 136.98	0.00 0.00 C _B) ₂) + (2 × C e rsc (unsub) = Residual 4.59	69SHI/MCN 69SHI/MCN C ₃ H ₁ C-(H) ₂ (C)(C _D)) +) Reference
$(8 \times C_8 - (1 \times C_8 $	H)(C _B) ₂) + corr) + (1 > Literatur 170.50 78.50 240.60 racyclophar H)(C _B) ₂) + corr) + (1 > Literatur 218.40	78.50 240.60 170.50 78.50 240.60 18e (4 × C _B -(C)(C _B) (2,2-Metaparac)	0.00 0.00 0.00 0.00 0.2) + (4 × C-(1) yclophane rse	H) ₂ (C)(C _B)) + Reference 69SHI/MCN 69SHI/MCN 69SCH/MCN C ₁₆ H ₁₆ H) ₂ (C)(C _B)) + c) Reference	Solid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Indane $(4 \times C_{B} - (\ell + \ell))$ Gas Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ Liquid Phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$ $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = \Delta_{\ell}S^{\circ} =$ $\Delta_{\ell}S^{\circ} = \Delta_{\ell}G^{\circ} =$	26.15 324.26 H)(C _B) ₂) + (1) ₂ (C) ₂) + (1 Literature 60.90	26.15 324.26 22 × C _{BI} – (C _{BI})(× Cyclopententer – Calculated = 56.31 102.02 10.40 170.16 279.95 – 424.56 136.98	0.00 0.00 C _B) ₂) + (2 × C e rsc (unsub) = Residual 4.59	69SHI/MCN 69SHI/MCN C,H, C-(H) ₂ (C)(C _D)) +) Reference

TABLE 13. Cyclic CH-02 (48) - Continued

TABLE 14. Cyclic CH-03 (47)

)(C))+(1	2×C _{BF} -(C _{BF}) ×C-(H) ₂ (C _d) ₂)		C_9H_8 C_d – $(H)(C_d))+$	Bicyclo[1.1.0 (2×C-(H) (1×Bicycl	$_{2}(C)_{2})+(2$	\times C-(H)(C) ₃) + ane rsc)	l	C₄H,
(1 × 1,5-0)	-	e – Calculated	= Residual	Reference	***	Literatur	e – Calculated =	= Residual	Reference
Gas Phase Δ _t H° =	163.30	165.19	-1.89	37DOL/GRE	Gas Phase $\Delta_f H^\circ =$	217.10	217.10	0.00	68WIB/FEN
Liquid Phase Δ _t H° =	110.42	117.05	-6.63	61STU/SIN	Liquid Phase $\Delta_t H^\circ =$	193.70	193.70	0.00	73SUN/WUL
					Bicyclopropy (4×C-(H)		× C-(H)(C) ₃) +	+ (2 × cyclopro	C ₆ H ₁ opane(sub) rsc)
						Literatur	e – Calculated =	= Residual	Reference
·					Gas Phase $\Delta_t H^\circ =$	129.40	127.04	2.36	66BEE/LUT
					Liquid Phase $\Delta_t H^\circ =$	95.90	80.70	15.20	66BEE/LUT
					Bicyclo[3.1.0 (4×C-(H) (1×Bicycl	$_{2}(C)_{2})+(2$	×C-(H)(C)₃)	-	C ₆ H ₁₀
						Literatur	e – Calculated =	= Residual	Reference
					Gas Phase $\Delta_t H^\circ =$	38.30	38.30	0.00	70CHA/MCN
					Liquid Phase $\Delta_t H^\circ =$	5.10	5.10	0.00	70CHA/MCN
		•			$(4 \times C_d - (H$	(C))+(2	diene; Norborn < C-(H)(C)(C _d) ta-2,5-diene rsc	$(1 \times C - (1 \times C - (1 \times C - (1 \times C + (1 \times C) + (1 \times C)))))))))))))))))))$	C7H8 H)2(C)2) +
		•				Literature	e – Calculated =	Residual	Reference
					Gas Phase $\Delta_f H^\circ =$	247.60	247.60	0.00	78STE4

Liquid Phase $\Delta_l H^\circ =$

213.80

213.80

0.00

78STE4

	$(C)_2 + (6)$	eptane; Quadri C-(H)(C) ₃) + '.0 ^{4,6}]heptane rs		C ₇ H ₈			×C-(H)(C) ₃) stane rsc)	+	С₁Н
	Literature	- Calculated =	Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas Phase $\Delta_i H^\circ =$	339.10	339.10	0.00	78STE4	Gas Phase Δ _t H° =	1.50	1.50	0.00	67BOY/SHI
Liquid Phase $\Delta_t H^\circ =$	302.10	302.10	0.00	78STE4	Liquid Phas Δ _t H° =	e -36.80	-36.80	0.00	67BOY/SHI
) ₂ (C) ₂) + (4) clo[2.2.1.0 ^{2,6}	ne × C-(H)(C) ₃) +]heptane rsc) :- Calculated =		C ₇ H ₁₀	(1 × Bicyc	() ₃ (C))+(4)	\times C-(H) ₂ (C) ₂) ane rsc) + (1 \times		C ₇ H ₁ C) ₃) +
				<u></u>		Literature	e – Calculated	= Residual	Reference
Gas Phase Δ _t II° –	82.10	82.10	0.00	78STE4	Gas Phase $\Delta_t H^\circ =$	1.50	11.85	- 10.35	71KOZ/TIM
Liquid Phas Δ _I H° –	e 43.40	43.40	0.00	78STE4	Liquid Phas				
	lo[2.2.1]hep	< C-(H) ₂ (C) ₂) + t-2-ene rsc) c – Calculated =			cis -1,2-Dieth				C ₇ H
			- Residual	Reference			$(C-(H)_2(C)_2)$ $(1 \times ci)$	+ (2 × C-(H)(s (unsat) corr	C) ₃) +
Gas Phase Δ _t H° =	91.20	91.20	0.00	78STE4		propane(sub		s (unsat) corr	C) ₃) +
$\Delta_t H^\circ =$						propane(sub	o) $rsc) + (1 \times ci$	s (unsat) corr	C) ₃) + ·)
$\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$	e	91.20			(1×cyclop	Propane(sub Literature	o) rsc)+(1×ci	s (unsat) corr	C) ₃) + ·)
Liquid Phase $\Delta_t H^\circ =$ Solid Phase $\Delta_t H^\circ =$ Bicyclo [2.2. (5 × C-(H	53.50	91.20 48.95 53.50 Norbornane × C-(H)(C) ₃) +	0.00	78STE4	Gas Phase $\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$ trans-1,2-Dia (2×C-(H	Literature e -79.90	- 37.95 - 80.10 opane < C-(H) ₂ (C) ₂)	es (unsat) corr	C) ₃) +) Reference 70LUP C ₇ H ₁
$\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$ Solid Phase $\Delta_t H^\circ =$ Bicyclo [2.2. (5 × C-(H)	53.50 1]heptane; ! 1) ₂ (C) ₂) + (2	91.20 48.95 53.50 Norbornane × C-(H)(C) ₃) +	0.00	78STE4 78STE4	Gas Phase $\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$ trans-1,2-Dia (2×C-(H	e e -79.90 ethylcyclopr () ₃ (C)) + (3) ₂ propane(sub	- 37.95 - 80.10 opane < C-(H) ₂ (C) ₂)	0.20 0.20	C) ₃) +) Reference 70LUP C ₇ H ₁
$\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$ Solid Phase $\Delta_t H^\circ =$ Bicyclo [2.2. (5 × C-(H) (1 × Bicyclo)	53.50 1]heptane; ! 1) ₂ (C) ₂) + (2	91.20 48.95 53.50 Norbornane × C-(H)(C) ₃) + tane rsc)	0.00	78STE4 78STE4 C ₇ H ₁₂	Gas Phase $\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$ trans-1,2-Dia (2×C-(H	e e -79.90 ethylcyclopr () ₃ (C)) + (3) ₂ propane(sub	- 37.95 - 80.10 opane < C-(H) ₂ (C) ₂)	0.20 0.20	C) ₃) +) Reference 70LUP C ₇ H ₁ C) ₃) +
$\Delta_t H^\circ =$ Liquid Phase $\Delta_t H^\circ =$ Solid Phase $\Delta_t H^\circ =$ Bicyclo[2.2. (5 × C-(H) (1 × Bicyclo) Gas Phase	53.50 1]heptane; ! 1] ₂ (C) ₂) + (2 2lo[2.2.1]hep Literature -61.60	91.20 48.95 53.50 Norbornane × C-(H)(C) ₃) + tane rsc) e - Calculated =	0.00 0.00	78STE4 78STE4 C ₇ H ₁₂ Reference	Gas Phase $\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$ $trans - 1, 2 - Dir (2 \times C - (H (1 \times cyclo)))$ Gas Phase	e -79.90 ethylcyclopr)3(C))+(3) propane(sub	o) rsc) + (1 × ci e - Calculated - 37.95 - 80.10 opane < C-(H) ₂ (C) ₂) o) rsc) e - Calculated	0.20 0.20	C) ₃) +) Reference 70LUP C ₇ H ₄ C) ₃) +

TABLE 14	Cyclic	CH-03	(47)	_	Continued
I ABLE 14.	L.VCHC	CD-03	(4/1	_	Continueu

octane rsc	$(C)_3) + (1 >$.0 ^{4,7}]octane; C Pentacyclo[4.2	ubane 2.0.0 ^{2,5} .0 ^{3,8} .0 ^{4,7}	C ₈ H ₈		$H)_2) + (1 \times 0)$	C _d -(H)(C))+(.×Cyclohexan		(C_d) +
W-1.67	Literature	e – Calculated =	Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas Phase Δ _t H° =	665.30	665.24	0.06	89KIR/CHU	Gas Phase $\Delta_t H^\circ = C_p^\circ =$	-48.90	-42.53 159.24	-6.37	79FUC/PEA
Solid Phase $\Delta_t H^\circ =$	585.00	585.00	0.00	89KIR/CHU	Liquid Phas $\Delta_l H^{\circ} = C_p^{\circ} =$	se - 88.70	- 82.93 208.98	- 5.77	61LAB/ROS
		× C-(H) ₂ (C) ₂) + 2-ene rsc)	- (2×C-(H)(C_8H_{12} $C)_2(C_d)) +$	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$		273.70 - 686.22 121.67 - 49.08		
	Literature	e – Calculated =	= Residual	Reference					
Gas Phase Δ _t H° =	20.50	20.50	0.00	70WON/WES		-	$2 \times C - (H)(C)_3$ ane rsc)	+	C ₈ H ₁₄
Solid Phase		ilia de Tre-				Literatur	e – Calculated	= Residual	Reference
$\Delta_{\rm f}H^{\circ} =$	-23.30	- 23.30	0.00	71WON/WES	Gas Phase $\Delta_l H^\circ =$	-25.40	25.40	0.00	70CHA/MCN
(1×C-(H	$H)_2)+(1\times C)$	C_{d} -(C) ₂) + (1 × C + (3 × C-(H) ₂ (C			Liquid Phas $\Delta_t H^\circ =$	e -68.20	68.20	0.00	70CHA/MCN
(1×C _d -(I (1×C-(H	$(H)_2) + (1 \times (1)_2) + (1 \times $	C_{d} -(C) ₂) + (1 × C + (3 × C-(H) ₂ (C	$(1 \times C - (1 \times C)))))))))))))))))))))))))))))))))))$	1))+	$\Delta_t H^\circ =$	-68.20	-68.20	0.00	
(1×C _d -(I (1×C-(H	$(H)_2) + (1 \times (1)_2) + (1 \times $	C_d - $(C)_2$) + $(1 \times C_d$ + $(3 \times C_d$ - $(H)_2$ (Cotane rsc)	$(1 \times C - (1 \times C)))))))))))))))))))))))))))))))))))$	(H)(C) ₃)+	$\Delta_t H^\circ =$ Bicyclo[5.1.6 $(6 \times C - (H))$	- 68.20 0]octane	:×C−(H)(C)₃)		70CHA/MCN C ₈ H ₁₄
$(1 \times C_d - (I \times C_d - (I \times C - (H \times C)))))))))))))))))$	H_{2}) + $(1 \times C)$ H_{2}) + $(1 \times C)$ H_{2} $H_$	C_d -(C) ₂) + (1 × 0 + (3 × C-(H) ₂ (C) otane rsc) e - Calculated =	$(1 \times C - (1 \times C)))))))))))))))))))))))))))))))))))$	(H)(C) ₃)+	$\Delta_t H^\circ =$ Bicyclo[5.1.6 $(6 \times C - (H))$	-68.20 0] octane 1)2(C)2) + (2 do[5.1.0] oct	:×C−(H)(C)₃)	+	
(1 × C _d -(I (1 × C-(H (1 × Bicyc	H_{2}) + $(1 \times C)$ H_{2}) + $(1 \times C)$ H_{2} $H_$	C_d -(C) ₂) + (1 × 0 + (3 × C-(H) ₂ (C) otane rsc) e - Calculated =	$(1 \times C - (1 \times C)))))))))))))))))))))))))))))))))))$	(H)(C) ₃)+	$\Delta_t H^\circ =$ Bicyclo[5.1.6 $(6 \times C - (H))$	-68.20 0] octane 1)2(C)2) + (2 do[5.1.0] oct	:×C-(H)(C) ₃) ane rsc)	+	C ₈ H ₁₄
$(1 \times C_d - (I \times C_d - (I \times C_d - (I \times C_d + (I \times Bicyc}))))$ Gas Phase $\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$ 2-Methylbic	H_{2}) + (1 × 0 H_{2}) + (1 × 0 H_{2}) (C ₂) (C ₄) · (1 H_{2}) (C ₂ 2.1] hep Literatur H_{2}	$\begin{array}{c} C_{d}^{-}(C)_2) + (1 \times C_{d}^{-}(C)_2) + (1 \times C_{d}^{-}(C)_2) + (1 \times C_{d}^{-}(C)_2) \\ + (3 \times C_{d}^{-}(C)_2) + (1 \times C_{d}^{-}(C)_2) + (1 \times C_{d}^{-}(C)_2) \\ + (3 \times C_$	2) ₂) + (1 × C-(= Residual 2.31	(H)(C) ₃) + Reference 69SKU/KOZ C ₈ H ₁₂	$\Delta_t H^\circ =$ Bicyclo[5.1.4 (6 × C-(H (1 × Bicyc) Gas Phase	-68.20 0] octane 1)2(C)2) + (2 10[5.1.0] oct Literature -16.70	× C-(H)(C) ₃) ane rsc) e – Calculated	+ = Residual	C ₈ H ₁₄ Reference
$(1 \times C_d - (H + C_d $	H_{2}) + $(1 \times C_{1})(C)_{2}$ + $(1 \times C_{2})(C)_{2}$ $(1 \times C_{2$	$C_{d}^{-}(C)_{2}^{-} + (1 \times C_{d}^{-}(C)_{2}^{-}) + (1 \times C_{d}^{-}(C)_{2$	$(C)_2) + (1 \times C - (C)_2) + (1 \times C - (C)_2) + (1 \times C_d - (C)_2) +$	69SKU/KOZ C ₈ H ₁₂ -(1×C _d -(H)(C))	Bicyclo [5.1.1] $(6 \times C - (H)$ $(1 \times Bicyc)$ Gas Phase $\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$	-68.20 O]octane ()2(C)2) + (2 do[5.1.0]oct Literature -16.70 e -60.30	- 16.70	+ = Residual 0.00	C ₈ H ₁₄ Reference 70CHA/MCN
$(1 \times C_d - (H + C_d $	$H_{12} + (1 \times C_{1})(C_{2}(C_{d})) + (1 \times C_{1})(C_{2}(C_{d})) + (1 \times C_{1})(C_{2}(C_{d})) + (1 \times C_{1})(C_{1}) + (1 \times C_{1})(C_{1}) + (1 \times C_{1})(C_{1})(C_{2}(C_{d}))$	$\begin{array}{c} C_{d}^{-}(C)_2) + (1 \times C_{d}^{-}(C)_2) + (1 \times C_{d}^{-}(C)_2) + (1 \times C_{d}^{-}(C)_2) \\ + (3 \times C_{d}^{-}(C)_2) + (1 \times C_{d}^{-}(C)_2) + (1 \times C_{d}^{-}(C)_2) \\ + (3 \times C_$	$(C)_{2} + (1 \times C - (C)_{2}) + (1 \times C - (C)_{2}) + (1 \times C_{3} - (C)_{2}) + (1 \times C_{3} - (C)_{2}) + (1 \times C_{3} - (C)_{2}) + (2.1] + (2.1) + (2$	69SKU/KOZ C ₈ H ₁₂ -(1×C _d -(H)(C))	Bicyclo [5.1.4] $(6 \times C - (H) + (1 \times Bicyc)$ Gas Phase $\Delta_t H^\circ = -\frac{1}{2}$ Liquid Phas $\Delta_t H^\circ = -\frac{1}{2}$ $cis - Bicyclo [3]$ $(6 \times C - (H) + (1 \times Bicyc)]$	-68.20 O]octane (1)2(C)2) + (2 fo[5.1.0]oct Literature -16.70 e -60.30	- 16.70 - 60.30 - X C-(H)(C) ₃)	+ = Residual 0.00	C ₈ H ₁₄ Reference 70CHA/MCN
$(1 \times C_d - (H_1)^2)$ $(1 \times C - (H_1)^2)$ Gas Phase $\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$ $2-Methylbic$ $(1 \times C - (H_1)^3)$ $(2 \times C - (H_2)^3)$	$H_{12} + (1 \times C_{1})(C_{2}(C_{d})) + (1 \times C_{1})(C_{2}(C_{d})) + (1 \times C_{1})(C_{2}(C_{d})) + (1 \times C_{1})(C_{1}) + (1 \times C_{1})(C_{1}) + (1 \times C_{1})(C_{1})(C_{2}(C_{d}))$	$C_{d}^{-}(C)_{2}^{-} + (1 \times C_{d}^{-}(C)_{2}^{-}) + (1 \times C_{d}^{-}(C)_{2}^{-}) + (1 \times C_{d}^{-}(C)_{2}^{-}) + (1 \times C_{d}^{-}(C)_{2}^{-}) + (1 \times Bicyclo[2$	$(C)_{2} + (1 \times C - (C)_{2}) + (1 \times C - (C)_{2}) + (1 \times C_{3} - (C)_{2}) + (1 \times C_{3} - (C)_{2}) + (1 \times C_{3} - (C)_{2}) + (2.1] + (2.1) + (2$	(1) + (2)	Bicyclo [5.1.4] $(6 \times C - (H) + (1 \times Bicyc)$ Gas Phase $\Delta_t H^\circ = -\frac{1}{2}$ Liquid Phas $\Delta_t H^\circ = -\frac{1}{2}$ $cis - Bicyclo [3]$ $(6 \times C - (H) + (1 \times Bicyc)]$	-68.20 Oloctane (1)2(C)2) + (2 Io[5.1.0]octa Literature -16.70 e -60.30 3.3.0]octane (2)2(C)2) + (2 (2)2(C)3.3.0]	- 16.70 - 60.30 - X C-(H)(C) ₃)	+ = Residual 0.00 0.00	C ₈ H ₁₄ Reference 70CHA/MCN
$(1 \times C_d - (H + C_d $	H_{2}) + (1 × C H_{2}) (C) ₂ (C _d)) + (1 × C H_{2}) (C) ₂ (C _d)) + (1 × C H_{2}) Literatur H_{2} H_{2} H_{2} H_{3} H_{2} H_{3	$C_{d}^{-}(C)_{2}^{-} + (1 \times C_{d}^{-}(C)_{2}^{-}) + (1 \times C_{d}^{-}(C)_{2}^{-}) + (1 \times C_{d}^{-}(C)_{2}^{-}) + (1 \times C_{d}^{-}(C)_{2}^{-}) + (1 \times Bicyclo[2$	$(C)_{2} + (1 \times C - (C)_{2}) + (1 \times C - (C)_{2}) + (1 \times C_{3} - (C)_{2}) + (1 \times C_{3} - (C)_{2}) + (1 \times C_{3} - (C)_{2}) + (2.1] + (2.1) + (2$	(1) + (2)	Bicyclo [5.1.4] $(6 \times C - (H) + (1 \times Bicyc)$ Gas Phase $\Delta_t H^\circ = -\frac{1}{2}$ Liquid Phas $\Delta_t H^\circ = -\frac{1}{2}$ $cis - Bicyclo [3]$ $(6 \times C - (H) + (1 \times Bicyc)]$	-68.20 Oloctane (1)2(C)2) + (2 Io[5.1.0]octa Literature -16.70 e -60.30 3.3.0]octane (2)2(C)2) + (2 (2)2(C)3.3.0]	- 16.70 - 60.30 (** C-(H)(C) ₃)	+ = Residual 0.00 0.00	C ₈ H ₁₄ Reference 70CHA/MCN 70CHA/MCN C ₈ H ₁₄

TABLE 14.	Cyclic CH-03	(47) -	Continued
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TABLE 14. Cyclic CH-03 (47) — Continued	TABLE 1	14.	Cyclic	CH-03	(47)	_	Continued
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				C 11	T 1 1 1 TO				
rans -Bicyclo	-			C ₈ H ₁₄	Liquid Phase				
$(6 \times C - (H))$	$_{12}(C)_{2})+(2)$	× C-(H)(C)3) +	+		$\Delta_{\rm f}H^{\circ} = -195.10$		- 8.83	71G00	
(1×trans-F	Bicyclo[3.3.0	O]octane)			$C_p^{\circ} =$	214.08			
					S° =	304.99			
	Literature	- Calculated =	≈ Residual	Reference	$\Delta_{\mathbf{f}}S^{\circ} =$	- 785.50			
					$\Delta_t G^\circ =$	47.93			
					$lnK_f =$	- 19.33			
Gas Phase									
	-66.60	-66.60	0.00	70CHA/MCN					
p. 2									
	-				cis-1-Ethyl-3-methy				C ₈ H ₁₆
Liquid Phase	:				$(2 \times C - (H)_3(C)) -$	$+(4\times C-(H)_2(C)_2)$	+(2×C-(H)((C) ₃) +	
$\Delta_i H^\circ = -$		- 109.20	0.00	70CHA/MCN		ertiary)) + $(1 \times Cy)$			
					Liter	ature – Calculated	= Residual	Reference	:
1-Methylbicy				C ₈ H ₁₄					
		$(C-(C)_4)+(1\times$		quaternary))+					
		$(C-(H)_2(C)_2)+$	ŀ		Gas Phase				
(1 × Bicycle	o[4.1.0]hep	tane rsc)			$\Delta_{\rm f}H^{\circ} =$	- 152.09			
					$C_p^{\circ} =$	155.31			
	Literature	- Calculated =	= Residual	Reference					·
					T !! 4 P!				
					Liquid Phase				
Gas Phase					$\Delta_{\rm f} H^{\rm o} = -194.40$		-8.13	71GOO	
$\Delta_{\rm f}H^{\circ} =$	-20.80	- 24.95	4.15	71KOZ/TIM	$C_p^{\circ} =$	214.08			
					S° =	304.99			
					$\Delta_{i}S^{\circ} =$	<i>−</i> 785.50			
Liquid Phase	e				$\Delta_t G^{\circ} =$	47.93			
$\Delta_t H^\circ =$	-59.90	- 66.04	6.14	71KOZ/TIM	$lnK_f =$	- 19.33			
cis-1-Ethyl-2 (2×C-(H)) ₃ (C))+(4>	opentane < C-(H) ₂ (C) ₂) - ary)) + (1 × Cyc				$+(4\times C-(H)_2(C)_2)$		(C) ₃) +	C ₈ H ₁₆
cis -1-Ethyl-2 (2×C-(H)) ₃ (C))+(4> corr (tertia	$< C-(H)_2(C)_2 > -$	lopentane (si	C) ₃)+	(2×C-(H) ₃ (C)) - (1×Cyclopentan		-CH ₃ corr (te	(C) ₃) +	
cis-1-Ethyl-2 (2×C-(H) (1×-CH ₃) ₃ (C))+(4> corr (tertia	$(C-(H)_2(C)_2) + (1 \times Cyc)$	lopentane (si	C) ₃) + ub) rsc)	(2×C-(H) ₃ (C)) - (1×Cyclopentan	$+ (4 \times C - (H)_2(C)_2)$ e (sub) rsc) + (1 ×	-CH ₃ corr (te	C) ₃) + ertiary))	
cis-1-Ethyl-2 (2×C-(H) (1×-CH ₃) ₃ (C))+(4> corr (tertia	< C-(H) ₂ (C) ₂) - ary)) + (1 × Cyc e – Calculated =	lopentane (si	C) ₃) + ub) rsc)	(2 × C-(H) ₃ (C)) - (1 × Cyclopentan	$+ (4 \times C - (H)_2(C)_2)$ e (sub) rsc) + (1 ×	-CH ₃ corr (te	C) ₃) + ertiary))	
cis-1-Ethyl-2 $(2 \times C - (H)$ $(1 \times -CH_3)$ Gas Phase $\Delta_t H^\circ =$) ₃ (C))+(4> corr (tertia	< C-(H) ₂ (C) ₂) + ary)) + (1 × Cyci e – Calculated = – – 152.09	lopentane (si	C) ₃) + ub) rsc)	(2 × C-(H) ₃ (C))- (1 × Cyclopentan Litera Gas Phase	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature – Calculated	-CH ₃ corr (te	C) ₃) + ertiary))	
cis-1-Ethyl-2 (2×C-(H) (1×-CH ₃) ₃ (C))+(4> corr (tertia	< C-(H) ₂ (C) ₂) - ary)) + (1 × Cyc e – Calculated =	lopentane (si	C) ₃) + ub) rsc)	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentan)$ Liter: Gas Phase $\Delta_l H^\circ =$	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature – Calculated – 152.09	-CH ₃ corr (te	C) ₃) + ertiary))	
cis -1-Ethyl-2 $(2 \times C - (H)$ $(1 \times -CH_3)$ Gas Phase $\Delta_t H^\circ =$) ₃ (C))+(4> corr (tertia	< C-(H) ₂ (C) ₂) + ary)) + (1 × Cyci e – Calculated = – – 152.09	lopentane (si	C) ₃) + ub) rsc)	(2 × C-(H) ₃ (C))- (1 × Cyclopentan Litera Gas Phase	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature – Calculated	-CH ₃ corr (te	C) ₃) + ertiary))	
Gas Phase $ \Delta_t H^\circ = C_p^\circ = Liquid Phase $) ₃ (C)) + (4> corr (tertia Literature	< C-(H) ₂ (C) ₂) + ary)) + (1 × Cyci e - Calculated = -152.09 155.31	lopentane (si	C) ₃) + ub) rsc) Reference	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentan)$ Liter: $Gas\ Phase$ $\Delta_t H^\circ = C_\rho^\circ =$	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature – Calculated – 152.09	-CH ₃ corr (te	C) ₃) + ertiary))	
Gas Phase $ \Delta_t H^\circ = C_p^\circ = $ Liquid Phase $ \Delta_t H^\circ = C_p^\circ = $) ₃ (C)) + (4> corr (tertia Literature	<pre>CC-(H)₂(C)₂) + Ary)) + (1 × Cycle c - Calculated = -152.09 155.31 -186.27</pre>	lopentane (si	C) ₃) + ub) rsc)	$(2 \times C - (H)_3(C))$ - $(1 \times Cyclopentan)$ Liters Gas Phase $\Delta_t H^\circ = C_\rho^\circ = C_\rho^$	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature – Calculated - 152.09 155.31	-CH ₃ corr (te	C) ₃) + ertiary)) Reference	
Gas Phase $\Delta_t H^\circ = C_p^\circ = $) ₃ (C)) + (4> corr (tertia Literature	CC-(H) ₂ (C) ₂) + (1 × Cyci ary)) + (1 × Cyci c - Calculated = -152.09 155.31 -186.27 214.08	lopentane (si	C) ₃) + ub) rsc) Reference	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentan)$ $Liters$ $Gas Phase$ $\Delta_l H^\circ = C_l^\circ =$ $Liquid Phase$ $\Delta_l H^\circ = -196.00$	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature - Calculated - 152.09 155.31	-CH ₃ corr (te	C) ₃) + ertiary))	
Gas Phase $C_{\rho}^{c} = \frac{1 - \text{Ethyl-2}}{(1 \times - \text{CH}_3)}$ Gas Phase $C_{\rho}^{t} = \frac{1 - \text{C}}{(1 \times - \text{CH}_3)}$ Liquid Phase $C_{\rho}^{t} = \frac{1 - \text{C}}{(1 \times - \text{C})^{t}}$ $C_{\rho}^{t} = \frac{1 - \text{C}}{(1 \times - \text{C})^{t}}$) ₃ (C)) + (4> corr (tertia Literature	CC-(H) ₂ (C) ₂) + (1 × Cyci ary)) + (1 × Cyci c - Calculated = -152.09 155.31 -186.27 214.08 304.99	lopentane (si	C) ₃) + ub) rsc) Reference	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentan)$ $Liters$ $Gas Phase$ $\Delta_t H^\circ = C_\rho^\circ =$ $Liquid Phase$ $\Delta_t H^\circ = -196.00$ $C_\rho^\circ =$	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature – Calculated - 152.09 155.31 0 - 186.27 214.08	-CH ₃ corr (te	C) ₃) + ertiary)) Reference	
Gas Phase $ \Delta_t H^\circ = C_p^\circ = $ Liquid Phase $ \Delta_t H^\circ = C_p^\circ = $) ₃ (C)) + (4> corr (tertia Literature	CC-(H) ₂ (C) ₂) + (1 × Cyci ary)) + (1 × Cyci c - Calculated = -152.09 155.31 -186.27 214.08	lopentane (si	C) ₃) + ub) rsc) Reference	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentan)$ $Liters$ $Gas Phase$ $\Delta_l H^\circ = C_l^\circ =$ $Liquid Phase$ $\Delta_l H^\circ = -196.00$	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature - Calculated - 152.09 155.31	-CH ₃ corr (te	C) ₃) + ertiary)) Reference	
Gas Phase $C_{\rho}^{c} = \frac{C_{\rho}^{c}}{C_{\rho}^{c}}$ Liquid Phase $C_{\rho}^{c} = \frac{C_{\rho}^{c}}{C_{\rho}^{c}} = \frac{C_{\rho}^{c}}{C_{\rho}^{c}} = \frac{C_{\rho}^{c}}{S_{\rho}^{c}} = \frac{C_{\rho}^{c}}{S_{\rho}^{c$) ₃ (C)) + (4> corr (tertia Literature	CC-(H) ₂ (C) ₂) + (1 × Cyci ary)) + (1 × Cyci c - Calculated = -152.09 155.31 -186.27 214.08 304.99	lopentane (si	C) ₃) + ub) rsc) Reference	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentan)$ $Liters$ $Gas Phase$ $\Delta_t H^\circ = C_\rho^\circ =$ $Liquid Phase$ $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ =$ $\Delta_t S^\circ =$	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature – Calculated - 152.09 155.31 0 - 186.27 214.08	-CH ₃ corr (te	C) ₃) + ertiary)) Reference	
Gas Phase $ \Delta_t H^\circ = C_p^\circ = $ Liquid Phase $ \Delta_t H^\circ = C_p^\circ = $) ₃ (C)) + (4> corr (tertia Literature	CC-(H) ₂ (C) ₂) + (1 × Cyci ary)) + (1 × Cyci c - Calculated = -152.09 155.31 -186.27 214.08 304.99 -785.50	lopentane (si	C) ₃) + ub) rsc) Reference	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentan)$ $Liters$ $Gas Phase$ $\Delta_l H^\circ = C_l^\circ =$ $Liquid Phase$ $\Delta_l H^\circ = -196.00$ $C_l^\circ = S^\circ =$	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature – Calculated - 152.09 155.31 0 - 186.27 214.08 304.99	-CH ₃ corr (te	C) ₃) + ertiary)) Reference	
Gas Phase $ \begin{array}{c} C_{p} = C_{p$) ₃ (C)) + (4> corr (tertia Literature	CC-(H) ₂ (C) ₂) + (1 × Cycle xy)) + (1 × Cycle xy)) + (1 × Cycle xy) + (1	lopentane (si	C) ₃) + ub) rsc) Reference	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentan)$ $Liters$ $Gas Phase$ $\Delta_t H^\circ = C_\rho^\circ =$ $Liquid Phase$ $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ =$ $\Delta_t S^\circ =$	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature – Calculated - 152.09 155.31 0 - 186.27 214.08 304.99 - 785.50	-CH ₃ corr (te	C) ₃) + ertiary)) Reference	
Gas Phase $\Delta_t H^\circ = C_p^\circ = $ Liquid Phase $\Delta_t H^\circ = C_p^\circ = $ $\Delta_t S^\circ = \Delta_t S^\circ = $ $\ln K_t = $) ₃ (C)) + (4> corr (tertia Literature	CC-(H) ₂ (C) ₂) + (1 × Cyci e-Calculated = -152.09 155.31 -186.27 214.08 304.99 -785.50 47.93 -19.33	lopentane (si	C) ₃) + µb) rsc) Reference 71GOO	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentan)$ $Liters$ $Gas Phase$ $\Delta_t H^\circ = C_\rho^\circ =$ $Liquid Phase$ $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature – Calculated - 152.09 155.31 0 - 186.27 214.08 304.99 - 785.50 47.93	-CH ₃ corr (te	C) ₃) + ertiary)) Reference	
Gas Phase $\Delta_t H^\circ = C_p^\circ = $ Liquid Phase $\Delta_t H^\circ = C_p^\circ = $ $\Delta_t S^\circ = \Delta_t S^\circ = $ $\Delta_t G^\circ = $ $\ln K_t = $ $trans - 1 - Ethy$) ₃ (C)) + (4> corr (tertia Literature e - 190.80	CC-(H) ₂ (C) ₂) + (1 × Cyci e-Calculated = -152.09 155.31 -186.27 214.08 304.99 -785.50 47.93 -19.33	e Residual	C) ₃) + 1b) rsc) Reference 71GOO	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentan)$ $Liters$ $Gas Phase$ $\Delta_t H^\circ = C_\rho^\circ =$ $Liquid Phase$ $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature – Calculated - 152.09 155.31 0 - 186.27 214.08 304.99 - 785.50 47.93	-CH ₃ corr (te	C) ₃) + ertiary)) Reference	
Gas Phase $ \Delta_t H^\circ = C_p^\circ = $ Liquid Phase $ \Delta_t H^\circ = C_p^\circ = $ $ \Delta_t S^\circ = \Delta_t S^\circ = $ $ \Delta_t G^\circ = $ $ \ln K_t = $ trans-1-Ethy $ (2 \times C - (H) $) ₃ (C)) + (4) corr (tertia Literature e - 190.80	CC-(H) ₂ (C) ₂) + (1 × Cyci e-Calculated = -152.09 155.31 -186.27 214.08 304.99 -785.50 47.93 -19.33 yelopentane × C-(H) ₂ (C) ₂)-	- 4.53	C) ₃) + 1b) rsc) Reference 71GOO C ₈ H ₁₆ C) ₃) +	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentan)$ $Liters$ $Gas Phase$ $\Delta_t H^\circ = C_\rho^\circ =$ $Liquid Phase$ $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	+ (4×C-(H) ₂ (C) ₂) e (sub) rsc) + (1× ature – Calculated - 152.09 155.31 0 - 186.27 214.08 304.99 - 785.50 47.93	-CH ₃ corr (te	C) ₃) + ertiary)) Reference	
Gas Phase $ \Delta_t H^\circ = C_p^\circ = $ Liquid Phase $ \Delta_t H^\circ = C_p^\circ = $ $ \Delta_t S^\circ = \Delta_t S^\circ = $ $ \Delta_t G^\circ = $ $ \ln K_t = $ trans-1-Ethy $ (2 \times C - (H) $) ₃ (C)) + (4) corr (tertia Literature e - 190.80	CC-(H) ₂ (C) ₂) + (1 × Cyci e-Calculated = -152.09 155.31 -186.27 214.08 304.99 -785.50 47.93 -19.33	- 4.53	C) ₃) + 1b) rsc) Reference 71GOO C ₈ H ₁₆ C) ₃) +	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentan)$ $Liters$ $Gas Phase$ $\Delta_t H^\circ = C_\rho^\circ =$ $Liquid Phase$ $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	- 152.09 155.31 - 186.27 214.08 304.99 - 785.50 47.93 - 19.33	-CH ₃ corr (te	C) ₃) + ertiary)) Reference	
Gas Phase $ \Delta_t H^\circ = C_p^\circ = $ Liquid Phase $ \Delta_t H^\circ = C_p^\circ = $ $ \Delta_t S^\circ = \Delta_t S^\circ = $ $ \Delta_t G^\circ = $ $ \ln K_t = $ trans-1-Ethy $ (2 \times C - (H) $	e - 190.80 1-2-methylc (3)(C)) + (4) corr (tertia	CC-(H) ₂ (C) ₂) + (1 × Cyc) e - Calculated = -152.09 155.31 -186.27 214.08 304.99 -785.50 47.93 -19.33 yclopentane × C-(H) ₂ (C) ₂) - ary)) + (1 × Cyc)	- 4.53 + (2×C-(H))(lopentane (st	C) ₃) + 1b) rsc) Reference 71GOO C ₃ H ₁₆ C) ₃) + 1b) rsc)	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentam)$ Liter: Gas Phase $\Delta_t H^\circ = C_\rho^\circ =$ Liquid Phase $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ 1-Ethyl-1-methylcyc	- 152.09 155.31 - 186.27 214.08 304.99 - 785.50 47.93 - 19.33	-CH ₃ corr (te	C) ₃) + ertiary)) Reference	
Gas Phase $ \Delta_t H^\circ = C_\rho^\circ = $ Liquid Phase $ \Delta_t H^\circ = C_\rho^\circ = $ $ \Delta_t S^\circ = \Delta_t S^\circ = $ $ \Delta_t G^\circ = $ $ \ln K_t = $ trans-1-Ethy $ (2 \times C - (H) $	e - 190.80 1-2-methylc (3)(C)) + (4) corr (tertia	CC-(H) ₂ (C) ₂) + (1 × Cyci e-Calculated = -152.09 155.31 -186.27 214.08 304.99 -785.50 47.93 -19.33 yelopentane × C-(H) ₂ (C) ₂)-	- 4.53 + (2×C-(H))(lopentane (st	C) ₃) + 1b) rsc) Reference 71GOO C ₈ H ₁₆ C) ₃) +	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentam)$ $Liters$ $Gas Phase$ $\Delta_t H^\circ = C_\rho^\circ = C_\rho^$	- 152.09 155.31 - 186.27 214.08 304.99 - 785.50 47.93 - 19.33	-CH ₃ corr (te = Residual -9.73	C) ₃) + ertiary)) Reference 71GOO	
Gas Phase $ \Delta_t H^\circ = C_\rho^\circ = $ Liquid Phase $ \Delta_t H^\circ = C_\rho^\circ = $ $ \Delta_t S^\circ = \Delta_t S^\circ = $ $ \Delta_t G^\circ = $ $ \ln K_t = $ trans-1-Ethy $ (2 \times C - (H) $	e - 190.80 1-2-methylc (3)(C)) + (4) corr (tertia	CC-(H) ₂ (C) ₂) + (1 × Cyc) e - Calculated = -152.09 155.31 -186.27 214.08 304.99 -785.50 47.93 -19.33 yclopentane × C-(H) ₂ (C) ₂) - ary)) + (1 × Cyc)	- 4.53 + (2×C-(H))(lopentane (st	C) ₃) + 1b) rsc) Reference 71GOO C ₃ H ₁₆ C) ₃) + 1b) rsc)	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentam)$ $Liters$ $Gas Phase$ $\Delta_t H^\circ = C_\rho^\circ =$ $Liquid Phase$ $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ = S^\circ = A_t S^\circ = A_t G^\circ = InK_t =$ $1-Ethyl-1-methylcyc$ $(2 \times C - (H)_3(C)) + (1 \times -CH_3 corr (C))$	- 152.09 - 155.31 - 186.27 - 214.08 - 304.99 - 785.50 - 47.93 - 19.33 - 19.33	-CH ₃ corr (te = Residual -9.73 + (1×C-(C) ₄)	C) ₃) + ertiary)) Reference 71GOO	C ₆ H ₁₆
Gas Phase $ \Delta_{t}H^{\circ} = C_{p}^{\circ} = $ Liquid Phase $ \Delta_{t}H^{\circ} = C_{p}^{\circ} = $ $ \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = $ $ \ln K_{t} = $ $ trans-1-Ethy $ $ (2 \times C-(H) $ $ (1 \times -CH_{3}) $ Gas Phase	e - 190.80 1-2-methylc (3)(C)) + (4) corr (tertia	CC-(H) ₂ (C) ₂) + (1 × Cyci e-Calculated = -152.09 155.31 -186.27 214.08 304.99 -785.50 47.93 -19.33 yclopentane × C-(H) ₂ (C) ₂) - ary)) + (1 × Cyci e-Calculated =	- 4.53 + (2×C-(H))(lopentane (st	C) ₃) + 1b) rsc) Reference 71GOO C ₃ H ₁₆ C) ₃) + 1b) rsc)	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentam)$ $Liters$ $Gas Phase$ $\Delta_t H^\circ = C_\rho^\circ =$ $Liquid Phase$ $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ = S^\circ = A_t S^\circ = A_t G^\circ = InK_t =$ $1-Ethyl-1-methylcyc$ $(2 \times C - (H)_3(C)) + (1 \times -CH_3 corr (C))$	- 152.09 155.31 - 186.27 214.08 304.99 - 785.50 47.93 - 19.33	-CH ₃ corr (te = Residual -9.73 + (1×C-(C) ₄)	C) ₃) + ertiary)) Reference 71GOO	C ₄ H ₁₆
Gas Phase $ \Delta_{t}H^{\circ} = C_{p}^{\circ} = $ Liquid Phase $ \Delta_{t}H^{\circ} = C_{p}^{\circ} = $ $ \Delta_{t}G^{\circ} = InK_{f} = $ trans-1-Ethy $ (2 \times C - (H_{1} \times CH_{3}) + CH_{3} \times CH_{3}) $	e - 190.80 1-2-methylc (3)(C)) + (4) corr (tertia	CC-(H) ₂ (C) ₂) + (1 × Cycle - Calculated = -152.09	- 4.53 + (2×C-(H))(lopentane (st	C) ₃) + 1b) rsc) Reference 71GOO C ₃ H ₁₆ C) ₃) + 1b) rsc)	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentam)$ $Liters$ $Gas Phase$ $\Delta_t H^\circ = C_\rho^\circ =$ $Liquid Phase$ $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ = S^\circ = A_t S^\circ = A_t G^\circ = InK_t =$ $1-Ethyl-1-methylcyc$ $(2 \times C - (H)_3(C)) + (1 \times -CH_3 corr (C))$	- 152.09 - 155.31 - 186.27 - 214.08 - 304.99 - 785.50 - 47.93 - 19.33 - 19.33	-CH ₃ corr (te = Residual -9.73 + (1×C-(C) ₄)	C) ₃) + ertiary)) Reference 71GOO	C ₄ H ₁₆
Gas Phase $ \Delta_{t}H^{\circ} = C_{p}^{\circ} = $ Liquid Phase $ \Delta_{t}H^{\circ} = C_{p}^{\circ} = $ $ \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = $ $ \ln K_{t} = $ $ trans-1-Ethy $ $ (2 \times C-(H) $ $ (1 \times -CH_{3}) $ Gas Phase	e - 190.80 1-2-methylc (3)(C)) + (4) corr (tertia	CC-(H) ₂ (C) ₂) + (1 × Cyci e-Calculated = -152.09 155.31 -186.27 214.08 304.99 -785.50 47.93 -19.33 yclopentane × C-(H) ₂ (C) ₂) - ary)) + (1 × Cyci e-Calculated =	- 4.53 + (2×C-(H))(lopentane (st	C) ₃) + 1b) rsc) Reference 71GOO C ₃ H ₁₆ C) ₃) + 1b) rsc)	$(2 \times \text{C-(H)}_{3}(\text{C})) - (1 \times \text{Cyclopentand})$ Liter: Gas Phase $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = C_{\rho}^$	- 152.09 - 155.31 - 186.27 - 214.08 - 304.99 - 785.50 - 47.93 - 19.33 - 19.33	-CH ₃ corr (te = Residual -9.73 + (1×C-(C) ₄)	C) ₃) + ertiary)) Reference 71GOO	C ₄ H ₁₆
Gas Phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \frac{\Delta_{t}G^{\circ}}{\ln K_{t}} = \frac{\Delta_{t}G^{\circ}}{\ln X_{t}} = \frac{\Delta_{t}G^$	e - 190.80 T-2-methylc; (3)(C)) + (4) corr (tertial Literature	CC-(H) ₂ (C) ₂) + (1 × Cycle - Calculated = -152.09	- 4.53 + (2×C-(H))(lopentane (st	C) ₃) + 1b) rsc) Reference 71GOO C ₃ H ₁₆ C) ₃) + 1b) rsc)	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentance)$ Liter: Gas Phase $\Delta_t H^\circ = C_\rho^\circ =$ Liquid Phase $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = 100$ $\Delta_t G^\circ = 100$ $1 - Ethyl-1 - methylcyc(2 \times C - (H)_3(C)) + (1 \times - CH_3 \text{ corr (of Literal Case Phase)})$ Gas Phase	- 152.09 155.31 - 186.27 214.08 304.99 - 785.50 47.93 - 19.33 - 19.33	-CH ₃ corr (te = Residual -9.73 + (1×C-(C) ₄)	C) ₃) + ertiary)) Reference 71GOO	C ₄ H ₁₆
Gas Phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = Liquid Phase$ $\Delta_{t}H^{\circ} = C_{p}^{\circ} = Liquid Phase$ $\Delta_{t}G^{\circ} = Liquid Phase$	e - 190.80 T-2-methylc; (3)(C)) + (4) corr (tertial Literature	CC-(H) ₂ (C) ₂) + (1 × Cycle - Calculated = -152.09	- 4.53 + (2×C-(H))(lopentane (st	C) ₃) + 1b) rsc) Reference 71GOO C ₃ H ₁₆ C) ₃) + 1b) rsc)	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentam)$ Liter: Gas Phase $\Delta_t H^\circ = C_\rho^\circ =$ Liquid Phase $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ 1-Ethyl-1-methylcyc $(2 \times C - (H)_3(C)) + (1 \times -CH_3 \text{ corr } (G))$ Liter: Gas Phase $\Delta_t H^\circ =$	- 152.09 155.31 - 186.27 214.08 304.99 - 785.50 47.93 - 19.33 - 19.33 - 19.33	-CH ₃ corr (te = Residual -9.73 + (1×C-(C) ₄)	C) ₃) + ertiary)) Reference 71GOO	C ₆ H ₁₆
Gas Phase $ \Delta_{t}H^{\circ} = C_{p}^{\circ} = Liquid Phase $ $ \Delta_{t}H^{\circ} = C_{p}^{\circ} = Liquid Phase $ $ \Delta_{t}G^{\circ} = Liquid Phase $	acorr (tertial Literature Literature e - 190.80 1-2-methylc; (3)(C)) + (4); corr (tertial	CC-(H) ₂ (C) ₂) + (1 × Cyci e - Calculated = -152.09 155.31 -186.27 214.08 304.99 -785.50 47.93 -19.33 -19.33 -19.33 -19.33 -19.33 -19.33	- 4.53 + (2×C-(H))(lopentane (si	C) ₃) + 1b) rsc) Reference 71GOO C ₃ H ₁₆ C) ₃) + 1b) rsc) Reference	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentance)$ Liter: Gas Phase $\Delta_t H^\circ = C_\rho^\circ =$ Liquid Phase $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = 100$ $\Delta_t G^\circ = 100$ $1 - Ethyl-1 - methylcyc(2 \times C - (H)_3(C)) + (1 \times - CH_3 \text{ corr (of Literal Case Phase)})$ Gas Phase	- 152.09 155.31 - 186.27 214.08 304.99 - 785.50 47.93 - 19.33 - 19.33	-CH ₃ corr (te = Residual -9.73 + (1×C-(C) ₄)	C) ₃) + ertiary)) Reference 71GOO	C ₆ H ₁₆
Gas Phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = Liquid Phase$ $\Delta_{t}H^{\circ} = C_{p}^{\circ} = Liquid Phase$ $\Delta_{t}G^{\circ} = Liquid Phase$	e - 190.80 Literature 1-2-methylc; corr (tertia	CC-(H) ₂ (C) ₂) + (1 × Cycle - Calculated = -152.09	- 4.53 + (2×C-(H))(lopentane (si	C) ₃) + 1b) rsc) Reference 71GOO C ₃ H ₁₆ C) ₃) + 1b) rsc) Reference	$(2 \times C - (H)_3(C)) - (1 \times Cyclopentam)$ Liter: Gas Phase $\Delta_t H^\circ = C_\rho^\circ =$ Liquid Phase $\Delta_t H^\circ = -196.00$ $C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ 1-Ethyl-1-methylcyc $(2 \times C - (H)_3(C)) + (1 \times -CH_3 \text{ corr } (G))$ Liter: Gas Phase $\Delta_t H^\circ =$	- 152.09 155.31 - 186.27 214.08 304.99 - 785.50 47.93 - 19.33 - 19.33 - 19.33	-CH ₃ corr (te = Residual -9.73 + (1×C-(C) ₄)	C) ₃) + ertiary)) Reference 71GOO	C ₆ H ₁₆

TABLE 14. Cyclic CH-03 (47) - Continued

(2×C-(H)	$_{3}(C))+(5\times$	ntane (Continu C-(H) ₂ (C) ₂) + rnary)) + (1 × 0	$-(1\times C-(C)_4)$		(2×C-(F	•	clo[2.2.1]hepta: \times C-(H) ₂ (C) ₂) ptane rsc)		C ₉ H ₁₀
	Literature	- Calculated =	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid Phase $\Delta_t H^\circ = \cdots = C_p^\circ = S^\circ =$		-186.68 211.98	- 7.12	71G00	Gas Phase $\Delta_t H^\circ =$	- 107.50	- 107.20	-0.30	70VAR/BEL
$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		286.50 - 803.99 53.03 - 21.39			Liquid Phas $\Delta_t H^\circ =$		-146.10	-4.10	71KOZ/TIM
Phenylcyclo	propane			C ₉ H ₁₀	7,7-Dimethy	ylbicyclo[2.2	2.1]heptane		C ₂ H ₁₆
(2×C-(H	$(C)_2 + (5)$	$\times C_B$ -(H)(C _B) ₂ -(1 × cycloprop		$C)(C_B)_2) +$	(2×-CH	(C) + (4 × corr (quantities) + (1.2.2.1]hep	ternary))+	2×C-(H)(C)	s)+(1×C-(C) ₄)+
	Literature	- Calculated =	= Residual	Reference			re – Calculated	= Residual	Reference
Gas Phase $\Delta_t H^\circ =$	150.50	152.86	-2.36	82FUC/HAL	Gas Phase $\Delta_l H^\circ =$		-115.41		
Liquid Phas	е	00.00	1.04	61KOS/LUK	Liquid Phas	se.			
$\Delta_t H^{\circ} =$	100.30	99.26	1.04	UIROS/LOR	$\Delta_t H^o =$		- 153.08		
$\Delta_i H^\circ =$ $cis-Bicyclo[6]$ $(7 \times C-(H))$	5.1.0]nonan	e × C-(H)(C) ₃) +		C ₉ H ₁₆	$\Delta_t H^\circ =$ Solid Phase		- 153.08 - 162.30	14.10	75KOZ/BYC
$\Delta_i H^\circ =$ $cis-Bicyclo[6]$ $(7 \times C-(H))$	5.1.0] nonand () ₂ (C) ₂) + (2 icyclo[6.1.0]	e × C-(H)(C) ₃) +	+		$\Delta_t H^\circ =$ Solid Phase $\Delta_t H^\circ =$ Bicyclo[3.3.	- 148.20 1]nonane	- 162.30		75KOZ/BYC C ₉ H ₁₆
$\Delta_t \dot{H}^\circ = {cis - Bicyclo[6]}$ $cis - Bicyclo[6]$	5.1.0] nonand () ₂ (C) ₂) + (2 icyclo[6.1.0]	e × C-(H)(C) ₃) - nonane rsc)	+	C ₉ H ₁₆	$\Delta_t H^\circ =$ Solid Phase $\Delta_t H^\circ =$ Bicyclo[3.3. $(7 \times C - (H^\circ))^{-1}$	- 148.20 1]nonane	-162.30 2×C-(H)(C)₃)-		
$\Delta_t H^\circ =$ cis -Bicyclo[t $(7 \times C - (H (1 \times cis$ -Bi Cis -Bi Cis -Bi Cis -Bi Cis -Bi Cis -Bi	6.1.0]nonane ()2(C)2) + (2 icyclo[6.1.0]i Literature -31.20	e × C-(H)(C) ₃) - nonane rsc) - Calculated =	+ = Residual	C ₉ H ₁₆ Reference	$\Delta_t H^\circ =$ Solid Phase $\Delta_t H^\circ =$ Bicyclo[3.3. $(7 \times C - (H^\circ))^{-1}$	-148.20 1]nonane 1] ₂ (C) ₂) + (2 elo[3.3.1]non	-162.30 2×C-(H)(C)₃)-	+	
$\Delta_t H^\circ =$ cis -Bicyclo[t $(7 \times C - (H (1 \times cis$ -Bi Gas Phase $\Delta_t H^\circ =$	6.1.0]nonane ()2(C)2) + (2 icyclo[6.1.0]i Literature -31.20	e × C-(H)(C) ₃) - nonane rsc) - Calculated =	+ = Residual	C ₉ H ₁₆ Reference	$\Delta_t H^\circ =$ Solid Phase $\Delta_t H^\circ =$ Bicyclo[3.3. $(7 \times C - (H^\circ))^{-1}$	- 148.20 1] nonane H) ₂ (C) ₂) + (2 elo[3.3.1] non Literatur	-162.30 2×C-(H)(C) ₃)	+	C ₃ H ₁₆
$\Delta_t H^\circ =$ cis -Bicyclo[4 $(7 \times C - (H (1 \times cis$ -Bi Gas Phase $\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$ $trans - (+)$ -B $(7 \times C - (H (1 \times cis + H (1 \times H (1$	5.1.0] nonance (2(C) ₂) + (2 (c) ₂ (c) ₁ (c) ₁ (c) ₁ (c) ₁ (c) ₂ (c) ₂	- XC-(H)(C) ₃) + nonane rsc) - Calculated = -31.20 - 80.30	+ Residual 0.00 0.00	C ₂ H ₁₆ Reference 78COR/PER	Solid Phase $\Delta_t H^\circ =$ Bicyclo[3.3. (7×C-(H (1×Bicyclose)) Gas Phase $\Delta_t H^\circ =$ Solid Phase	- 148.20 1] nonane H) ₂ (C) ₂) + (2 elo[3.3.1] non Literatur - 127.50	- 162.30 2×C-(H)(C) ₃)- nane rsc) re - Calculated	+ = Residual	C ₉ H ₁₆ Reference
$\Delta_t H^\circ =$ cis -Bicyclo[4 $(7 \times C - (H (1 \times cis$ -Bi Gas Phase $\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$ $trans - (+)$ -B $(7 \times C - (H (1 \times cis + H (1 \times H (1$	5.1.0] nonano (1)2(C)2) + (2 (2) (2) (6.1.0] Literature -31.20 se -80.30 icyclo[6.1.0] (1)2(C)2) + (2 -Bicyclo[6.1.0]	- XC-(H)(C) ₃) - nonane rsc) - Calculated = - 31.20 - 80.30 nonane × C-(H)(C) ₃) -	+ Residual 0.00 0.00	C ₂ H ₁₆ Reference 78COR/PER	Solid Phase $\Delta_{t}H^{\circ} = \frac{1}{2}$ Bicyclo[3.3. $(7 \times C - (F + (1 \times Bicyc)))$ Gas Phase $\Delta_{t}H^{\circ} = \frac{1}{2}$ Solid Phase $\Delta_{t}H^{\circ} = \frac{1}{2}$	- 148.20 1]nonane 1) ₂ (C) ₂) + (2 clo[3.3.1]non Literatur - 127.50	-162.30 2 × C-(H)(C) ₂)-nane rsc) re - Calculated = -127.50 -178.20	+ = Residual 0.00	C ₃ H ₁₆ Reference 77PAR/STE 77PAR/STE
$\Delta_t H^\circ =$ cis -Bicyclo[4 $(7 \times C - (H (1 \times cis$ -Bi Gas Phase $\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$ $trans - (+)$ -B $(7 \times C - (H (1 \times cis + H (1 \times H (1$	5.1.0] nonano (1)2(C)2) + (2 (2) (2) (6.1.0] Literature -31.20 se -80.30 icyclo[6.1.0] (1)2(C)2) + (2 -Bicyclo[6.1.0]	- XC-(H)(C) ₃) - nonane rsc) - Calculated = - 31.20 - 80.30 nonane × C-(H)(C) ₃) - 0]nonane rsc)	+ Residual 0.00 0.00	C ₉ H ₁₆ Reference 78COR/PER 78COR/PER	Solid Phase $\Delta_{t}H^{\circ} = \frac{1}{2}$ Bicyclo[3.3. $(7 \times C - (H + 1) \times H) \times (1 \times H)$ Gas Phase $\Delta_{t}H^{\circ} = \frac{1}{2}$ Solid Phase $\Delta_{t}H^{\circ} = \frac{1}{2}$ Cyclopentyle $(9 \times C - (H + 1) \times H) \times (9 \times C - (H + 1) \times H)$	- 148.20 1]nonane H) ₂ (C) ₂) + (2 elo[3.3.1]non Literatur - 127.50 - 178.20 cyclohexane H) ₂ (C) ₂) + (2	-162.30 2 × C-(H)(C) ₂)-nane rsc) re - Calculated = -127.50 -178.20	+ Residual 0.00 0.00	C ₉ H ₁₆ Reference 77PAR/STE 77PAR/STE C ₁₁ H ₂₆
$\Delta_t H^\circ =$ cis-Bicyclo[t] $(7 \times C - (H (1 \times cis - Bi)))$ Gas Phase $\Delta_t H^\circ =$ Liquid Phas $\Delta_t H^\circ =$ trans-(+)-B $(7 \times C - (H (1 \times trans)))$ Gas Phase	6.1.0]nonane ()2(C)2) + (2) (cyclo[6.1.0]) Literature -31.20 (e) -80.30 (icyclo[6.1.0]) (1)2(C)2) + (2 (2) (3) (4) (5) (5) (6.1.0] (7) (7) (8) (9) (9) (9) (1) (1) (1) (2) (2) (2) (3) (4) (4) (5) (6) (6) (7) (7) (7) (7) (7) (7) (7) (7) (7) (7	e × C-(H)(C) ₃) - nonane rsc) e - Calculated = -31.20 -80.30 nonane × C-(H)(C) ₃) - 0]nonane rsc) e - Calculated =	+ Residual 0.00 0.00 + Residual	C ₉ H ₁₆ Reference 78COR/PER 78COR/PER C ₉ H ₁₆	Solid Phase $\Delta_{t}H^{\circ} = \frac{1}{2}$ Bicyclo[3.3. $(7 \times C - (H + 1) \times H) \times (1 \times H)$ Gas Phase $\Delta_{t}H^{\circ} = \frac{1}{2}$ Solid Phase $\Delta_{t}H^{\circ} = \frac{1}{2}$ Cyclopentyle $(9 \times C - (H + 1) \times H) \times (9 \times C - (H + 1) \times H)$	- 148.20 1]nonane H) ₂ (C) ₂) + (2 elo[3.3.1]non Literatur - 127.50 - 178.20 cyclohexane t) ₂ (C) ₂) + (2 epentane (s	-162.30 2×C-(H)(C) ₃)- nane rsc) re - Calculated = -127.50 -178.20	Residual 0.00 0.00	C ₉ H ₁₆ Reference 77PAR/STE 77PAR/STE C ₁₁ H ₂₆

Cyclopentylcyclohexane (Continued) $(9 \times C - (H)_2(C)_2) + (2 \times C - (H)(C)_3) + (1 \times Cyclopentane (sub) rsc) + (1 \times Cyclohexane (sub) rsc) + (1 \times Cyclohex$	C ₁₁ H ₂₀ b) rsc)	Heptylcyclohexane $(1 \times C - (H)_3(C)) + (11 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2) + (1$	$C_{13}H_{26}$ $H)(C)_3) +$	
Literature – Calculated = Residual	Reference	Literature – Calculated = Residual	Reference	
Liquid Phase $\Delta_t H^\circ = -230.20 -219.58 -10.62$ $C_p^\circ = 267.01$ $S^\circ = 325.39$	61KOZ/SKU	Gas Phase $\Delta_t H^\circ = -289.20 -270.75 -18.45$ $C_p^\circ = 274.78$	78FUC/PEA	
$\Delta_t S^\circ = -1043.46$ $\Delta_t G^\circ = 91.53$ $\ln K_t = -36.92$		Liquid Phase $\Delta_t H^\circ = -353.00 -337.47 -15.53$ $C_p^\circ = 366.27$	40MOO/REN	
Cyclopentylcycloheptane $ (10 \times C - (H)_2(C)_2) + (2 \times C - (H)(C)_3) + \\ (1 \times Cyclopentane (sub) rsc) + (1 \times Cycloheptane rsc) + (1 \times Cycloheptan$	C ₁₂ H ₂₂	$S^{\circ} = 440.69$ $\Delta_{f}S^{\circ} = -1331.35$ $\Delta_{f}G^{\circ} = 59.47$ $\ln K_{f} = -23.99$		
Literature - Calculated = Residual Gas Phase	Reference	Bicyclohexyl $(10 \times C \cdot (H)_2(C)_2) + (2 \times C - (H)(C)_3) + (2 \times Cyclohexane (sub) rsc)$	C ₁₂ H ₂₂	
$\Delta_t H^\circ = -162.75$ $C_p^\circ = 204.05$	· .	Literature – Calculated = Residual	Reference	
Liquid Phase $\Delta_t H^\circ = -226.30 -219.75 -6.55$ $C_p^\circ - 291.45$ $S^\circ = 348.56$	61KOZ/SKU	Gas Phase $\Delta_{i}H^{\circ} = -215.70 -209.42 -6.28$ $C_{\rho}^{\circ} - 223.42$	78MON/ROS	
$\Delta_t S^\circ = -1156.60$ $\Delta_t G^\circ = 125.09$ $\ln K_t = -50.46$		Liquid Phase $\Delta_t H^\circ = -273.70 -270.96 -2.74$ $C_p^\circ = 294.54$	76GOO/LEE	
Dicyclopentylmethane $(9 \times C - (H)_2(C)_2) + (2 \times C - (H)(C)_3) + (2 \times C)_2(C)_2(C)_2(C)_3(C)_3(C)_3(C)_3(C)_3(C)_3(C)_3(C)_3$	C ₁₁ H ₂₀	$S^{\circ} = 326.22$ $\Delta_{i}S^{\circ} = -1178.94$ $\Delta_{i}G^{\circ} = 80.54$ $\ln K_{f} = -32.49$		
Literature – Calculated = Residual	Reference	Bicycloheptyl	C ₁₄ H ₂₆	
Gas Phase $\Delta_t H^{\circ} = -148.91$ $C_p^{\circ} = 190.43$		$(12 \times C - (H)_2(C)_2) + (2 \times C - (H)(C)_3) + (2 \times Cyclobe$ $Literature - Calculated = Residual$	Reference	
Liquid Phase $\Delta_t H^{\circ} = -205.10 -193.93 -11.17$ $C_p^{\circ} = 269.90$	61KOZ/SKU	Gas Phase $\Delta_{\nu}H^{\circ} = -197.22$ $C_{p}^{\circ} = 240.56$		
$S^{\circ} = 356.94$ $\Delta_t S^{\circ} = -1011.91$ $\Delta_t G^{\circ} = 107.77$ $\ln K_t = -43.47$		Liquid Phase $\Delta_t H^\circ = -285.00 -271.30 -13.70$ $C_p^\circ = 343.42$ $S^\circ = 372.56$	61KOZ/SKU	
		$\Delta_t S^\circ = -1405.22$ $\Delta_t G^\circ = 147.67$ $\ln K_t = -59.57$		

TARIE '	14	Cyclic	CH-03	(47)	_	Continued
IABLE	14.	CACHE	C11-03	(4/)	_	Continued

	$H)(C_B)_2$ +	ne (2×C _B -(C)(C +(1×cycloproj			9,9'-Bianthr (18×C _B -($(2 \times C_B - (C_B)(C_B))$	(B _F) ₂) + (8×0	$C_{28}H_{16}$ C_{BF} – $(C_{BF})(C_B)_2)$
(2 ~ C -(11)	,	e – Calculated :		Reference		Literatur	e – Calculated =	Residual	Reference
Gas Phase					Gas Phase $\Delta_t H^\circ =$	454.30	454.30	0.00	58HOY/PEP
$\Delta_{\mathfrak{g}}H^{\circ} =$		261.66					-11 - 14		
Liquid Phase Δ _f H° =	178.80	179.13	-0.33	61KOZ/LUK	Solid Phase $\Delta_f H^\circ =$	326.20	326.20	0.00	51MAG/HAR
	$H)(C_B)_2) +$	pane (2×C _B -(C)(C + (1×cyclopro				(H)(C _B) ₂) +	$(2 \times C_B - (C_B)_2)$ culated = Residu	,, .	$C_{28}H_{1}$ C_{BF} – $(C_{BF})(C_{B})_2)$ ence
	Literatur	e – Calculated	= Residual	Reference	Solid Phase $\Delta_t H^{\circ} =$	212.80	212.80	0.00	51MAG/HAR
Gas Phase $\Delta_t H^{\circ} =$		261.66							
Liquid Phase Δ _i H° =	e 166.20	179.13	- 12.93	61KOZ/LUK		$C)(C_B)_2)+($	30 × C _B -(H)(C _B		
	$I(C_d) + (2$	yl-1,3-butadien 2×C _d -(H)(C _B)		C ₁₆ H ₁₄ d)(C _B) ₂) +	Solid Phase $\Delta_t H^\circ =$	511.80	511.80	0.00	36BEN/CUT2
	Literatur	e – Calculated	= Residual	Reference	1,1,4,4-Tetra			\. \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	C ₂₈ H ₂₄
Gas Phase					(20 × C _B -((2 × C-(H		$(2 \times C - (H)_2(C))$	2) + (4 × C _B -	(C)(C _B) ₂) +
$\Delta_t H^\circ = C_p^\circ =$		299.56 238.50					culated = Residu	ıal Refere	ence
Liquid Phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	e	208.56 372.36 323.82 682.02 411.90 166.16			Liquid Phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \operatorname{In} K_t = S^\circ = $	•	145.44 577.84 620.40 - 1237.74 514.47 - 207.53		
Solid Phase $\Delta_t H^\circ = C_r^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	178.80	175.96 303.90 294.50 -711.34 388.05 -156.53	2.84	53COO/HO12	Solid Phase $\Delta_t H^\circ = C_p^\circ =$	163.30	160.18 440.50	3.12	53COO/HOI

TABLE 15. Alcohols (69)

$\begin{array}{l} \textbf{1,2'-Dinaphthylmethane} & C_{21}H_{16} \\ (1\times C-(H)_2(C_B)_2) + (2\times C_B-(C)(C_B)_2) + (4\times C_{BF}-(C_{BF})(C_B)_2) + \\ (14\times C_B-(H)(C_B)_2) \end{array}$						
	Literatur	e – Calculated =	Reference			
Gas Phase						
$\Delta_i H^\circ =$		274.59				
Liquid Phas	se .					
$\Delta_{i}H^{\circ} =$		189.38				
$C_p^{\circ} =$		408.71				
<i>s</i> ° =		394.99				
$\Delta_f S^\circ =$		-770.12				
$\Delta_f G^\circ =$		418.99				
$lnK_f =$		- 169.02				
Solid Phase	:					
$\Delta_t H^\circ =$	162.00	154.18	7.82	78GOO		
$C_n^{\circ} =$		313.56				
S° =		306.35				
$\Delta_f S^\circ =$		-858.76				
$\Delta_t G^\circ =$		410.22				
$\ln K_{\rm f} =$		- 165.48				

	Literature	- Calculated -	- Residual	Reference
Gas Phase	;			
$\Delta_f H^\circ =$	-201.10	201.59	0.49	32ROS
$C_0^{\circ} =$	43.89	43.89	0.00	69STU/WES
S° =	239.70	239.69	0.01	69STU/WES
$\Delta_f S^\circ =$		-129.72		
$\Delta_f G^\circ =$		- 162.91		
$lnK_f =$		65.72		
Liquid Ph	asc			
$\Delta_t H^\circ =$		-239.11	0.61	85MAJ/SVO
$C_p^{\circ} =$		81.12	0.01	71CAR/WES
S° =		127.19	0.00	71CAR/WES
$\Delta_t S^\circ =$		-242.21		
$\Delta_f G^\circ =$		- 166.89		
$lnK_f =$		67.32		

Ethanoi; Ethyl alcohol C_2H_6O $(1 \times C - (H)_3(C)) + (1 \times O - (H)(C)) + (1 \times C - (H)_2(O)(C)), \sigma = 3$ Literature – Calculated = Residual Reference

Gas Phase	e			
$\Delta_t H^\circ =$	-235.30	-234.49	-0.81	32ROS
$C_n^{\circ} = 0$	65.44	64.22	1.22	69STU/WES
<i>S</i> ° =	282.59	283.12	-0.53	69STU/WES
$\Delta_f S^\circ =$		-222.60		
$\Delta_t G^{\circ} =$		-168.12		
$lnK_f =$		67.82		
Liquid Ph	ase			
Liquid Ph $\Delta_t H^\circ =$	ase 277.60	- 274.91	- 2.69	85MAJ/SVO
•		- 274.91 114.76	- 2.69 - 2.26	85MAJ/SVO 77HAI/SUG
$\Delta_f H^\circ =$	-277.60			
$\Delta_{f}H^{\circ} = C_{p}^{\circ} =$	-277.60 112.50	114.76	-2.26	77HAI/SUG
$\Delta_t H^\circ = C_p^\circ = S^\circ =$	-277.60 112.50	114.76 159.78	-2.26	77HAI/SUG
$\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} =$	-277.60 112.50	114.76 159.78 - 345.93	-2.26	77HAI/SUG

	Literatui	re – Calculated	Reference	
Gas Phase	2			
$\Delta_t H^\circ =$	-124.50	-124.18	-0.32	38DOL/GRE
$C_p^{\circ} =$	76.02	76.02	0.00	69STU/WES
S° =	307.57	307.56	0.01	69STU/WES
$\Delta_t S^\circ =$		-203.89		
$\Delta_f G^\circ =$		-63.39		
$lnK_f =$		25.57		

TABLE 15. Alcohols (69) - Continued

TABLE 15. Alcohols (69) - Continued

$(1 \times C_{d}-($		ol (Continued) C _d -(H)(C))+(1	× C-(H) ₂ (O)	C ₃ H ₆ O (C _d))+	(1×C-(I	t-Pentyl alc H) ₃ (C))+(3 H)(C)), σ =	\times C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂	C ₅ H ₁₂ O (O)(C)) +
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid Pha $\Delta_t H^\circ = C_p^\circ =$	-171.10 138.91	-167.32 138.91	-3.78 0.00	49GEL/SKI 1881REI	Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	-294.70 132.88 402.54	- 296.38 132.89 400.60 - 514.05	1.68 - 0.01 1.94	66WAD2 69STU/WES 69STU/WES
(1×C-(n-Propyl alo H) ₃ (C))+(1 H) ₂ (O)(C)),	\times C-(H) ₂ (C) ₂)	+ (1 × O-(H)(C ₃ H ₈ O	$\Delta_f G^\circ = \\ \ln K_f = \\ -$		-143.12 57.73	,	
Gas Phase	Literatur	re – Calculated	= Residual	Reference	Liquid Pha $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = $	- 351.60 208.14 258.90	-352.10 206.02 256.92 -657.73	0.50 2.12 1.98	75MOS/DEK 68COU/LEE 68COU/LEE
$\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} =$	-255.10 87.11 324.80	-255.12 87.11 322.28 -319.75	0.02 0.00 2.52	61SNE/SKI 69STU/WES 69STU/WES	$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = \\ -$		-156.00 62.93		
$\Delta_t G^\circ = \ln K_t = \frac{1}{2}$	***	- 159.79 64.46			(1×C-(1	- Hexyl alco H) ₃ (C)) + (4 H)(C)), σ =	\times C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂	C ₆ H ₁₄ O (O)(C))+
Liquid Phate $\Delta_t H^\circ = C_t^\circ = S^\circ = C_t^\circ$	- 302.60 143.80 192.80	-300.64 145.18 192.16	-1.96 -1.38 0.64	61SNE/SKI 68COU/LEE 68COU/LEE		Literatu	re – Calculated	= Residual	Reference
$\Delta_{\rm f}S^{\circ} = \Delta_{\rm f}G^{\circ} = \ln K_{\rm f} = 0$		- 449.87 - 166.51 67.17			Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	-315.90 155.77 441.50	-317.01 155.78 439.76 -611.20	1.11 -0.01 1.74	66WAD2 69STU/WES 69STU/WES
(1×C-(- Butyl alcol (H) ₃ (C))+(2 (H)(C)), σ =	\times C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂	C ₄ H ₁₀ O	$\Delta_f G^\circ = \ln K_f =$		-134.78 -134.37		
Gas Phase	·	re - Calculated		Reference	Liquid Pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$	se - 377.50 242.50 287.40	-377.83 236.44 289.30 -761.66	0.33 6.06 -1.90	75MOS/DEK 89VES/BAR 29KEL
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	-275.01 110.00 363.17	- 275.75 110.00 361.44 - 416.90 - 151.45	0.74 0.00 1.73	66WAD2 69STU/WES 69STU/WES	$\Delta_f G^\circ = \\ \ln K_f = \\ -$		-150.74 60.81		
$lnK_f =$		61.09					\times C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂ (C ₇ H ₁₆ O (O)(C))+
Liquid Ph $\Delta_t H^\circ = C_p^\circ = S^\circ =$	- 327.20 177.16 225.70	- 326.37 175.60 224.54	-0.83 1.56 1.16	69MOS/DEK 65COU/HAL 65COU/HAL	- Amm	Literatur	re – Calculated	= Residual	Reference
$\Delta_{\rm f}S^{\circ} = \\ \Delta_{\rm f}G^{\circ} = \\ \ln K_{\rm f} = $		- 553.80 - 161.26 65.05			Gas Phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0 $	- 336.50 178.66 480.45	- 337.64 178.67 478.92 - 708.35 - 126.44 51.01	1.14 -0.01 1.53	77MAN/SEL 69STU/WES 69STU/WES

TABLE 15. Alcohols (69) - Continued

TABLE 15. Alcohols (69) - Continued

(1 × C-(H		ohol (Continue \times C-(H) ₂ (C) ₂) + 3		C ₇ H ₁₆ O (O)(C))+	(1×C-(1-Decyl alco H)3(C))+(8 (H)(C)), σ =	$3 \times C - (H)_2(C)_2$	+ (1 × C–(H) ₂	$C_{10}H_{22}O$ (O)(C))+
	Literatur	e – Calculated =	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid Phas	se				Gas Phase	;			
$\Delta_t H^{\circ} =$	-403.30	-403.56	0.26	75MOS/DEK	$\Delta_{\rm f}H^{\circ} =$	- 396.60	- 399.53	2.93	79SVE
$C_p^{\circ} =$	270.80	266.86	3.94	89VES/BAR	$C_p^{\circ} =$	247.32	247.34	-0.02	69STU/WES
S° =	325.90	321.68	4.22	56PAR/KEN	S° =	597.31	596.40	0.91	69STU/WES
$\Delta_{\rm f}S^{\circ} =$		- 865.59			$\Delta_f S^\circ =$		- 999.81		
$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = $		145.48 58.69			$\Delta_f G^\circ = \ln K_f =$		101.44 40.92		
							· 		
					Liquid Pha				
	Octyl alcoh			C ₈ H ₁₈ O	$\Delta_{\rm f}H^{\circ} =$	 478.10	-480.75	2.65	75MOS/DEK
, ,		\times C-(H) ₂ (C) ₂)	+ (1×C-(H) ₂	(O)(C))+	$C_p^{\circ} = S^{\circ} =$		358.12 418.82		
(1×0-(1	H)(C)), σ =	: 3			Δ ₆ 5° =		- 1177.38		
	Literatus	re – Calculated	= Residual	Reference	$\Delta_{\rm f}G^{\circ} =$		- 129.71		
		- Culculated			$\ln K_f =$		52.33		
Gas Phase									
$\Delta_{\rm f}H^{\circ} =$	-355.60	-358.27	2.67	77MAN/SEL					
$C_p^{\circ} =$	201.54	201.56	-0.02	69STU/WES	Undecanol				C ₁₁ H ₂₄ O
S° =	519.40	518.08	1.32	69STU/WES		H)3(C))+(9 H)(C)),	$0 \times C - (H)_2(C)_2$	$+(1\times C-(H)_2)$	(O)(C))+
$\Delta_f S^\circ = \Delta_f G^\circ =$		- 805.50 - 118.11			(1×0-(11)(0)), 0 -	- 3		
$lnK_f =$		47.64				Literatu	re – Calculated	= Residual	Reference
			 						
Liquid Pha		100.00	0.70	an toomer	Gas Phase		100.16	204	(0.000 t 0.000
$\Delta_i H^\circ =$	-426.50	-429.29	2.79 6.72	75MOS/DEK 89VES/BAR	$\Delta_{\rm f}H^{\circ} =$	- 422.20 270.20	- 420.16	- 2.04	69STU/WES
$C_p^{\circ} = S^{\circ} =$	304.00	297.28 354.06	0.72	09 V E3/DAK	$C_p^{\circ} = S^{\circ} =$	636.30	270.23 635.56	- 0.03 0.74	69STU/WES 69STU/WES
Δ ₁ S° =		- 969.52			Δ ₆ S° =	030.30	- 1096.96	0.74	09310/WE3
$\Delta_t G^\circ =$		- 140.23			$\Delta_{\rm f}G^{\circ} =$		- 93.10		
$\ln K_{\rm f} =$		56.57			$lnK_f =$		37.56		
					Liquid Pha	000			
Nonanol: n	-Nonyi alco	hol		C9H20	$\Delta_{\rm f}H^{\circ} =$	- 504.80	-506.48	1.68	75MOS/DEK
		\times C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂		$C_p^{\circ} =$	407.00	388.54	18.46	90ZAB/RUZ
	H)(C)), σ =		(, , , , , , , , , , , , , , , , , , ,	()())	S° =		451.20		7 3 7 . 7 . 7
• • •	, , ,,				$\Delta_f S^\circ =$		- 1281.31		
	Literatu	re – Calculated :	≈ Residual	Reference	$\Delta_{\mathbf{f}}G^{\circ} =$		- 124.46		
	· · · · · · · · · · · · · · · · · · ·		······		$lnK_f =$		50.20		
Gas Phase $\Delta_t H^\circ =$	- 375.50	270 nn	2 40	77M A NI/CEI					
$C_{\rho}^{\circ} =$	- 373.50 224.43	-378.90 224.45	3.40 0.02	77MAN/SEL 69STU/WES	Dodecanel	; n -Dodecyl	alcohol		C ₁₂ H ₂₆ O
$S^{\circ} =$	558.35	557.24	1.11	69STU/WES			$0 \times C - (H)_2(C)_2$	+(1×C-(H)	
$\Delta_i S^\circ =$	556.05	- 902.66	1.41	0202 O/ 17 MO		H)(C)), σ =		· (* ^ O-(11)	ヘンハンル・
$\Delta_{\rm f}G^{\circ} =$		-109.77			(2		-		
$\ln K_t -$		44.28				Literatu	re - Calculated	= Residuai	Reference
Liouid Dt.				-	Con Dha				
Liquid Pha	- 453.60	-455 M	1.42	75MOS/DEK	Gas Phase $\Delta_t H^{\circ} =$	-436.60	440 70	A 10	70\$3/P
	- 7JJ.UU	- 455.02 327.70	1.74	/JMOJ/DEK	$C_{\rho}^{\circ} =$	293.09	440.79 293.12	4.19 0.03	79SVE 69STU/WES
$\Delta_l II^{\circ}$ –		321.10							
$\Delta_l II^\circ - C_p^\circ =$		386.44			N° =	675.21	(174.77	().49	695111/WHS
$\Delta_t II^\circ - C_p^\circ = S^\circ =$		386.44 1073.45			$S^{\circ} = \Delta_{6}S^{\circ} =$	675.21	674.72 1194.11	0.49	69STU/WES
$\Delta_l II^\circ - C_p^\circ =$		386.44 1073.45 134.97			$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = 0$	6/5.21	- 1194.11 - 84.77	0.49	6951U/WES

TABLE 15. Alcohols (69) - Continued

Liquid Phase $ \Delta_t H^{\circ} = -C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = $		e – Calculated :	= Residual	D -f					
$ \Delta_t H^\circ = -C_p^\circ = S^\circ = -C_p^\circ = -C$				Reference		Literatu	re – Calculated	= Residual	Reference
$ \Delta_t H^\circ = -C_p^\circ = S^\circ = -C_p^\circ = -C$:				Liquid Pha	ise			
$C_p^{\circ} = S^{\circ} =$	- 528.50	-532.21	3.71	75MOS/DEK	$\Delta_t H^\circ =$	- 579.70	-583.67	3.97	91STE/CHI
s° =	438.30	418.96	19.34	90ZAB/RUZ	$C_p^{\circ} =$	575.70	479.80	5.57	JIDIL/CIII
	430.30		17.54	JULAD/KUL	$S^{\circ} =$				
$\Delta_{f}S^{\circ} =$		483.58			_		548.34		
		- 1385.24			$\Delta_f S^\circ =$		- 1593.11		
$\Delta_{\mathfrak{l}}G^{\circ} =$		- 119.20			$\Delta_f G^{\circ} =$		- 108.69		
$lnK_f =$		48.08			$lnK_f =$		43.84		
					Solid Phase	e			
Tridecanol; <i>n</i>	n -Tridecyl	alcohol		C ₁₃ H ₂₈ O	$\Delta_f H^\circ =$	-628.18	-632.32	4.14	91STE/CHI
		\times C-(H) ₂ (C) ₂)+(1×C-(H)		$C_p^{\circ} =$	388.00	381.66	6.34	74MOS/MOU
(1×O-(H)			(21)	2(0)(0))	$C_p^{\circ} =$	426.32	381.66	44.66	91STE/CHI
(17.0 (11)	//~/// · · ·	~			S° =	.25.02	386.16	. 1.00) IO I I OI II
	T 24 4 -	Colonia 1	_ D oc!d1	Dafa					•
	Literatur	e – Calculated	= Kesiduai	Reference	$\Delta_{f}S^{\circ} =$		- 1755.29		
					$\Delta_t G^{\circ} =$		- 108.98		
					$lnK_f =$		43.96		
Gas Phase									
$\Delta_{\mathbf{f}}H^{\circ} =$		- 461.42							
$C_p^{\circ} =$	315.85	316.01	-0.16	69STU/WES					
S° =	711.82	713.88	-2.06	69STU/WES	Pentadecar	nol; n-Penta	decyl alcohol		C ₁₅ H ₃₂
$\Delta_{\mathbf{f}}S^{\circ} =$		- 1291.26				•	$3 \times C - (H)_2(C)_2$)+(1×C-(H)	
$\Delta_{\mathbf{f}}G^{\circ} =$		-76.43				H)(C)), σ =) (1/10 (11)	2(0)(0)) !
					(1 × 0-()	11)(0)), 0 -	- ,		
$lnK_f =$		30.83				Literatu	re – Calculated	= Residual	Reference
Liquid Phase	e				·				
$\Delta_t H^\circ =$		557.94			Gas Phase				
$C_p^{\circ} =$		449.38			$\Delta_t H^\circ =$		-502.68		
$S^{\circ} =$		515.96			$C_p^{\circ} =$	361.58	361.79	-0.21	69STU/WES
									•
$\Delta_{\mathbf{f}}S^{\circ} =$		- 1489.18			S° =	790.73	792.20	-1.47	69STU/WES
$\Delta_{\rm f}G^{\circ} =$		- 113.94			$\Delta_f S^{\circ} =$		- 1485.56		
$lnK_f =$		45.96			$\Delta_f G^\circ = \ln K_f =$		-59.76 24.11		
Solid Phase									
$\Delta_t H^\circ = -$	- 599.40	- 602.91	3.51	75MOS/DEK	Liquid Pha	ise			
$C_p^{\circ} =$	378.00	359.74	18.26	74MOS/MOU	$\Delta_{\mathbf{f}}H^{\circ} =$		-609.40		
S° =		363.15			$C_p^{\circ} =$		510.22		
$\Delta_{\epsilon}S^{\circ} =$		- 1641.99			$S^{\circ} =$		580.72		
$\Delta_i G^\circ =$					$\Delta_f S^\circ =$		- 1697.04		
		-113.35							
$lnK_f =$		45.73			$\Delta_{\rm f}G^{\circ} =$		- 103.43		
					$lnK_f =$		41.72		
Tetradecano	ol; <i>n</i> -Tetrac	lecyl alcohol		C ₁₄ H ₃₀ O	Solid Phase	е			
		$2 \times C - (H)_2(C)_2$)+(1×C-(H)		$\Delta_f H^\circ =$	-658.20	- 661.73	3.53	75MOS/DEK
	I)(C)), σ =		()		$C_p^{\circ} =$	400.00	403.58	-3.58	74MOS/MOU
(2.00 (11	-,(~,), 0 -	-			$S^{\circ} =$		409.17	2,20	,
	T itamatu	re – Calculated	- Danidus	Deference					
	Literatu	e – Calculated	- Vezionsi	Reference	$\Delta_f S^\circ =$		- 1868. 5 9		
					$\Delta_f G^\circ = \ln K_f =$		- 104.61 42.20		
Gas Phase					••••••		12.20		
	- 474.80	- 482.05	7.25	91STE/CHI					
	338.74	338.90	-0.16						
$C_p^{\circ} =$				69STU/WES					
60	751.78	753.04	- 1.26	69STU/WES					
S° =		-1388.41							
$\Delta_f S^\circ =$									
		- 68.10							

) ₃ (C))+(1	ecyl alcohol; Co $4 \times C - (H)_2(C)_2$ = 3		C ₁₆ H ₃₄ O ₂ (O)(C))+			$6 \times C - (H)_2(C)_2$	2)+(1×C-(H	C ₁₈ H ₃₈ C) ₂ (O)(C)) +
	Literatu	re – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas Phase					Gas Phase				
	-517.00	-523.31	6.31	65DAV/KYB	$\Delta_{\rm f}H^{\circ} =$		-564.57		
$C_p^o =$	384.47	384.68	-0.21	69STU/WES	$C_p^{\circ} =$	430.20	430.46	-0.26	69STU/WES
S° =	829.69	831.36	-1.67	69STU/WES	S° =	907.59	909.68	- 2.09	69STU/WES
$\Delta_f S^\circ =$	027.07	- 1582.71	2.07		$\Delta_f S^\circ =$		- 1777.01		
$\Delta_{i}G^{\circ} =$		-51.42			$\Delta_{\rm f}G^{\circ} =$		-34.75		
$lnK_f =$		20.74			$lnK_f =$		14.02		
					7	***************************************			
Liquid Phas	е				Liquid Phas	e	606 5 0		
$\Delta_{\rm f}H^{\circ} =$		-635.13			$\Delta_{\rm f}H^{\circ} =$		-686.59		
$C_p^{\circ} =$		540.64			$C_p^{\circ} =$		601.48		
S° =		613.10			S° =		677.86		
$\Delta_f S^\circ =$		- 1800.97			$\Delta_f S^\circ =$		- 2008.83		
$\Delta_t G^{\circ} =$		-98.17			$\Delta_f G^\circ =$		-87.66		
$lnK_t =$		39.60			$lnK_f =$		35.36		
Solid Phase					Solid Phase				
	- 686.30	- 691.14	4.84	75MOS/DEK	$\Delta_t H^\circ =$		- 749.96		
$C_p^{\circ} =$	422.00	425.50	-3.50	74MOS/MOU	$C_p^{\circ} =$		469.34		
$S^{\circ} =$	722.00	432.18	3.30	741400/1400	S° =		478.20		
-					$\Delta_{\mathbf{f}}S^{\circ} =$		- 2208.49		
A C°					CIT				
$\Delta_{\rm f}S^{\circ} =$		- 1981.89			A C		_ 01 50		
$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = $	-	100.24 40.44			$\Delta_t G^\circ = \ln K_f = -$		-91.50 36.91		
$\Delta_f G^\circ = \ln K_f = \frac{1}{1 \times C - (H)}$	I) ₃ (C))+(1 I)(C)), σ	-100.24 40.44 adecyl alcohol 15 × C-(H) ₂ (C) ₂ = 3			$ \frac{\ln K_{\rm f} = }{\text{Nonadecano}} $ $ (1 \times C - (H_{\rm f})) = \frac{1}{2} \left(\frac{1}{2} \times \frac{1}{2} \right) \left(\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \right) \left(\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \right) \left(\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \right) \left(\frac{1}{2} \times \frac$	$I_{3}(C) + (1^{\circ})_{3}(C), \sigma =$	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂		
$\Delta_f G^\circ = \ln K_f = \frac{1}{1 \times C - (H)}$	I) ₃ (C))+(1 I)(C)), σ	-100.24 40.44 adecyl alcohol 15×C-(H) ₂ (C) ₂			$ \frac{\ln K_{\rm f} = }{\text{Nonadecano}} $ $ (1 \times C - (H_{\rm f})) = \frac{1}{2} \left(\frac{1}{2} \times \frac{1}{2} \right) \left(\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \right) \left(\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \right) \left(\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \right) \left(\frac{1}{2} \times \frac$	$I_{3}(C) + (1^{\circ})_{3}(C), \sigma =$	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂		
$\Delta_f G^\circ = \ln K_f = \frac{1}{1 \times C - (H)}$	I) ₃ (C))+(1 I)(C)), σ	-100.24 40.44 adecyl alcohol 15 × C-(H) ₂ (C) ₂ = 3		₂ (O)(C))+	$ \frac{\ln K_{\rm f} = }{\text{Nonadecano}} $ $ (1 \times C - (H_{\rm f})) = \frac{1}{2} \left(\frac{1}{2} \times \frac{1}{2} \right) \left(\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \right) \left(\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \right) \left(\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \right) \left(\frac{1}{2} \times \frac$	$I_{3}(C) + (1^{\circ})_{3}(C), \sigma =$	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂) ₂ (O)(C)) +
$\Delta_t G^\circ = \ln K_f = \frac{1 \times C - (H_f)}{1 \times C - (H_f)}$	I) ₃ (C))+(1 I)(C)), σ	-100.24 40.44 adecyl alcohol 15 × C-(H) ₂ (C) ₂ = 3		₂ (O)(C))+	Nonadecano (1×C-(H (1×O-(H	$I_{3}(C) + (1^{\circ})_{3}(C), \sigma =$	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂) ₂ (O)(C))+
$\Delta_f G^\circ = \ln K_f = \frac{1}{1}$ Heptadecan (1 × C-(H) (1 × O-(H) Gas Phase $\Delta_t H^\circ = \frac{1}{1}$	I) ₃ (C))+(1 I)(C)), σ	- 100.24 40.44 tadecyl alcohol 15 × C-(H) ₂ (C) ₂ = 3 ure - Calculated		₂ (O)(C))+	Nonadecand $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_{\ell} H^{\circ} =$	$I_{3}(C) + (1^{\circ})_{3}(C), \sigma =$	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ 3 re - Calculated) ₂ (O)(C)) + Reference
$\Delta_t G^\circ = \frac{1}{\ln K_f} = \frac{1}{\ln K_f}$ Heptadecan $(1 \times C - (H_f))$ $(1 \times O - (H_f))$ Gas Phase $\Delta_t H^\circ = C_t^\circ = S^\circ = C_t^\circ = S^\circ = C_t^\circ = C_t^\circ$	() ₃ (C)) + (1 (I)(C)), σ Literatu	- 100.24 40.44 tadecyl alcohol 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94	= Residual	Reference	Nonadecand $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	() ₃ (C)) + (1 I)(C)), σ = Literatur	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ 3 re – Calculated - 585.20	= Residual) ₂ (O)(C))+
$\Delta_t G^\circ = \frac{1}{\ln K_f} = \frac{1}{\ln K_f}$ Heptadecan $(1 \times C - (H_f))$ $(1 \times O - (H_f))$ Gas Phase $\Delta_t H^\circ = C_t^\circ = S^\circ = C_t^\circ = S^\circ = C_t^\circ = C_t^\circ$	(1) ₃ (C)) + (1 (1)(C)), σ = Literatu	- 100.24 40.44 40.44 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	(C) ₃ (C)) + (1 I)(C)), σ = Literatur 453.08	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ = 3 re - Calculated - 585.20 453.35	= Residual -0.27) ₂ (O)(C)) + Reference 69STU/WES
$\Delta_t G^\circ = \frac{1}{\ln K_t} = \frac{1}{\ln K_t}$ Heptadecan (1 × C-(H) (1 × O-(H) Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \frac{1}{\ln K_t}$	(1) ₃ (C)) + (1 (1)(C)), σ = Literatu	- 100.24 40.44 40.44 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = 0$	(C) ₃ (C)) + (1 I)(C)), σ = Literatur 453.08	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ = 3 re - Calculated - 585.20 453.35 948.84	= Residual -0.27) ₂ (O)(C)) + Reference 69STU/WES
$\Delta_t G^\circ = \frac{1}{\ln K_t} = \frac{1}{\ln K_t}$ Heptadecan $(1 \times C - (H_t))$ Gas Phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \frac{1}{\ln K_t}$	(1) ₃ (C)) + (1 (1)(C)), σ = Literatu	- 100.24 40.44 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	(C) ₃ (C)) + (1 I)(C)), σ = Literatur 453.08	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ 3 re - Calculated - 585.20 453.35 948.84 - 1874.17	= Residual -0.27	Reference 69STU/WES
$\Delta_t G^\circ = \ln K_t = \frac{1 \times C(H)}{1 \times C(H)}$ Heptadecan $(1 \times C(H))$ Gas Phase $\Delta_t H^\circ = C_t^\circ = S_t^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1 \times C(H)}{1 \times C(H)}$	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	-100.24 40.44 40.44 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated -543.94 407.57 870.52 -1679.86 -43.09	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ 3 re - Calculated - 585.20 453.35 948.84 - 1874.17 - 26.42	= Residual) ₂ (O)(C)) + Reference 69STU/WES
$\Delta_t G^\circ = \ln K_f = \frac{1 \times C(H)}{1 \times C(H)}$ Heptadecan $(1 \times C(H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S_0^\circ = \Delta_t G^\circ = \ln K_f = \frac{1 \times C(H)}{1 \times C(H)}$ Liquid Phas	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	- 100.24 40.44 ladecyl alcohol 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86 - 43.09 17.38	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = Liquid Phase$	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ 3 re - Calculated - 585.20 453.35 948.84 - 1874.17 - 26.42 10.66	= Residual) ₂ (O)(C)) + Reference 69STU/WES
$\Delta_t G^\circ = \ln K_f = \frac{1 \times C(H)}{1 \times C(H)}$ Heptadecan $(1 \times C(H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_f = \frac{1 \times C(H)}{1 \times C(H)}$ Liquid Phas $\Delta_t H^\circ = \frac{1 \times C(H)}{1 \times C(H)}$	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	- 100.24 40.44 tadecyl alcohol 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86 - 43.09 17.38	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{\Delta_t G^\circ}{\Delta_t H^\circ} = \frac{\Delta_t G^\circ}{\Delta_$	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ = 3 re - Calculated - 585.20 453.35 948.84 -1874.17 - 26.42 10.66	= Residual) ₂ (O)(C)) + Reference 69STU/WES
$\Delta_t G^\circ = \ln K_f = \frac{1}{100}$ Heptadecan (1 × C-(H) (1 × O-(F) Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_f = \frac{1}{100}$ Liquid Phas $\Delta_t H^\circ = C_p^\circ = $	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	- 100.24 40.44 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86 - 43.09 17.38 - 660.86 571.06	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{\Delta_t H^\circ}{\Delta_t H^\circ} = C_p^\circ =$	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ = 3 re - Calculated - 585.20 453.35 948.84 - 1874.17 - 26.42 10.66 - 712.32 631.90	= Residual) ₂ (O)(C)) + Reference 69STU/WES
$\Delta_t G^\circ = \ln K_t = \frac{1}{1 \times G^\circ}$ Heptadecan (1 × C-(H) (1 × O-(H) Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{1 \times G^\circ}$ Liquid Phas $\Delta_t H^\circ = C_p^\circ = S^\circ = $	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	- 100.24 40.44 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86 - 43.09 17.38 - 660.86 571.06 645.48	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{\Delta_t G^\circ = \ln K_t}{\Delta_t H^\circ = C_p^\circ = S^\circ = S^\circ = S^\circ = S^\circ = \Delta_t G^\circ = $	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ = 3 re - Calculated - 585.20 453.35 948.84 - 1874.17 - 26.42 10.66 - 712.32 631.90 710.24	= Residual) ₂ (O)(C)) + Reference 69STU/WES
$\Delta_t G^\circ = \ln K_t = \frac{1}{1 \times C(H_t)}$ Heptadecan $(1 \times C(H_t))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{1}{1 \times C_p^\circ}$ Liquid Phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \frac{1}{1 \times C_p^\circ}$	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	- 100.24 40.44 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86 - 43.09 17.38 - 660.86 571.06 645.48 - 1904.90	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \Delta_t G^\circ = \ln K_t = K_t^\circ = K$	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ = 3 re - Calculated - 585.20 453.35 948.84 - 1874.17 - 26.42 10.66 - 712.32 631.90 710.24 - 2112.76	= Residual) ₂ (O)(C)) + Reference 69STU/WES
$\Delta_t G^\circ = \ln K_t = \frac{1 \times G^\circ}{\ln K_t} = \frac{1 \times G^\circ}{\ln X \cdot G^\circ} = \frac{1 \times G^\circ}{\ln K_t} = $	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	- 100.24 40.44 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86 - 43.09 17.38 - 660.86 571.06 645.48	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{\Delta_t G^\circ = \ln K_t}{\Delta_t H^\circ = C_p^\circ = S^\circ = S^\circ = S^\circ = S^\circ = \Delta_t G^\circ = $	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ = 3 re - Calculated - 585.20 453.35 948.84 - 1874.17 - 26.42 10.66 - 712.32 631.90 710.24	= Residual	Reference 69STU/WES
$\Delta_t G^\circ = \ln K_f = \frac{1}{16}$ Heptadecan $(1 \times C - (H) + (1 \times C - (H))$ Gas Phase $\Delta_t H^\circ = C_t^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{16}$ Liquid Phase $\Delta_t H^\circ = C_t^\circ = \Delta_t G^\circ = \frac{1}{16}$ $\Delta_t H^\circ = C_t^\circ = \frac{1}{16}$	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	- 100.24 40.44 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86 - 43.09 17.38 - 660.86 571.06 645.48 - 1904.90 - 92.91	= Residual	Reference 69STU/WES	In K_f = Nonadecand $(1 \times C - (H) \times C - (H) \times C - (H) \times C - (H) \times C \times $	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ 3 re - Calculated - 585.20 453.35 948.84 - 1874.17 - 26.42 10.66 - 712.32 631.90 710.24 - 2112.76 - 82.40	= Residual) ₂ (O)(C)) + Reference 69STU/WES
$\Delta_t G^\circ = \ln K_f = \frac{1}{\sqrt{G^\circ}}$ Heptadecan $(1 \times C - (H) + (1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{\sqrt{G^\circ}}$ Liquid Phase $\Delta_t H^\circ = C_p^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t = \frac{1}{\sqrt{G^\circ}}$ Solid Phase	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	- 100.24 40.44 ladecyl alcohol 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86 - 43.09 17.38 - 660.86 571.06 645.48 - 1904.90 - 92.91 37.48	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(2 \times C - (H))$ $(3 \times C - (H))$ $(4 \times C - (H))$ $(5 \times C - (H))$ $(5 \times C - (H))$ $(6 \times C - (H))$ $(7 \times C - (H))$ $(7 \times C - (H))$ $(8 \times C - (H))$ $(8 \times C - (H))$ $(9 \times C - (H))$ $(9 \times C - (H))$ $(1 \times (H))$ $($	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ 3 re - Calculated - 585.20 453.35 948.84 - 1874.17 - 26.42 10.66 - 712.32 631.90 710.24 - 2112.76 - 82.40 33.24	= Residual	Reference 69STU/WES
$\Delta_t G^\circ = \ln K_f = \frac{1}{\sqrt{G^\circ}}$ Heptadecan $(1 \times C - (H) + (1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{\sqrt{G^\circ}}$ Liquid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{\sqrt{G^\circ}}$ Solid Phase $\Delta_t H^\circ = \frac{1}{\sqrt{G^\circ}}$	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	- 100.24 40.44 ladecyl alcohol 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86 - 43.09 17.38 - 660.86 571.06 645.48 - 1904.90 - 92.91 37.48	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(2 \times C - (H))$ $(3 \times C - (H))$ $(4 \times C - (H))$ $(5 \times C - (H))$ $(6 \times C - (H))$ $(7 \times C - (H))$ $(7 \times C - (H))$ $(8 \times C - (H))$ $(8 \times C - (H))$ $(9 \times C - (H))$ $(9 \times C - (H))$ $(1 \times (H))$	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ 3 re - Calculated - 585.20 453.35 948.84 - 1874.17 - 26.42 10.66 - 712.32 631.90 710.24 - 2112.76 - 82.40 33.24 - 779.37	= Residual	Reference 69STU/WES
$\Delta_t G^\circ = \ln K_f = \frac{1}{\sqrt{G^\circ}}$ Heptadecan $(1 \times C - (H) + (1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_f = \frac{1}{\sqrt{G^\circ}}$ Liquid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_f = \frac{1}{\sqrt{G^\circ}}$ Solid Phase $\Delta_t H^\circ = C_p^\circ = C_$	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	- 100.24 40.44 ladecyl alcohol 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86 - 43.09 17.38 - 660.86 571.06 645.48 - 1904.90 - 92.91 37.48	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(2 \times C - (H))$ $(3 \times C - (H))$ $(4 \times C - (H))$ $(5 \times C - (H))$ $(6 \times C - (H))$ $(7 \times C - (H))$ $(7 \times C - (H))$ $(8 \times C - (H))$ $(8 \times C - (H))$ $(9 \times C - (H))$ $(9 \times C - (H))$ $(1 \times $	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ 3 re - Calculated - 585.20 453.35 948.84 - 1874.17 - 26.42 10.66 - 712.32 631.90 710.24 - 2112.76 - 82.40 33.24 - 779.37 491.26	= Residual	Reference 69STU/WES
$\Delta_t G^\circ = \ln K_t = \frac{1}{\sqrt{G^\circ}}$ Heptadecan $(1 \times C - (H) + (1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{\sqrt{G^\circ}}$ Liquid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{\sqrt{G^\circ}}$ Solid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \frac{1}{\sqrt{G^\circ}}$	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	- 100.24 40.44 tadecyl alcohol 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86 - 43.09 17.38 - 660.86 571.06 645.48 - 1904.90 - 92.91 37.48	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{\Delta_t H^\circ}{\Delta_t H^\circ} = C_t^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t H^\circ = C_t^\circ = S^\circ =$	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ = 3 re - Calculated - 585.20 453.35 948.84 -1874.17 -26.42 10.66 - 712.32 631.90 710.24 -2112.76 -82.40 33.24 - 779.37 491.26 501.21	= Residual) ₂ (O)(C)) + Reference 69STU/WES
$\Delta_t G^\circ = \ln K_t = \frac{1}{\sqrt{G^\circ}}$ Heptadecan $(1 \times C - (H) + (1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{\sqrt{G^\circ}}$ Liquid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{\sqrt{G^\circ}}$ Solid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \frac{1}{\sqrt{G^\circ}}$	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	- 100.24 40.44 ladecyl alcohol 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86 - 43.09 17.38 - 660.86 571.06 645.48 - 1904.90 - 92.91 37.48	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{\Delta_t H^\circ}{\Delta_t H^\circ} = C_t^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ =$	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ 3 re - Calculated - 585.20 453.35 948.84 - 1874.17 - 26.42 10.66 - 712.32 631.90 710.24 - 2112.76 - 82.40 33.24 - 779.37 491.26	= Residual	Reference 69STU/WES
$\Delta_t G^\circ = \ln K_t = \frac{1}{\sqrt{G^\circ}}$ Heptadecan $(1 \times C - (H) + (1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{\sqrt{G^\circ}}$ Liquid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{\sqrt{G^\circ}}$ Solid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \frac{1}{\sqrt{G^\circ}}$	(I) ₃ (C)) + (I I)(C)), σ = Literatu 407.35 868.64	- 100.24 40.44 tadecyl alcohol 15 × C-(H) ₂ (C) ₂ = 3 are - Calculated - 543.94 407.57 870.52 - 1679.86 - 43.09 17.38 - 660.86 571.06 645.48 - 1904.90 - 92.91 37.48	= Residual	Reference 69STU/WES	Nonadecand $(1 \times C - (H))$ $(1 \times C - (H))$ $(1 \times O - (H))$ Gas Phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{\Delta_t H^\circ}{\Delta_t H^\circ} = C_t^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t H^\circ = C_t^\circ = S^\circ =$	(l) ₃ (C)) + (1' I)(C)), σ = Literatur 453.08 946.55	36.91 lecyl alcohol 7 × C-(H) ₂ (C) ₂ = 3 re - Calculated - 585.20 453.35 948.84 -1874.17 -26.42 10.66 - 712.32 631.90 710.24 -2112.76 -82.40 33.24 - 779.37 491.26 501.21	= Residual) ₂ (O)(C)) + Reference 69STU/WES

TABLE 15. Alcohols (69) - Continued

	•	$8 \times C - (H)_2(C)_2$	+ (1 × C-(H)	C ₂₀ H ₄₂ O ₂ (O)(C))+		$H_{3}(C) + (1$	×C-(H) ₂ (C) ₂)		$C_5H_{12}O$ $C)_3) + (1 \times O - (H)(C))$
(2.1.0 (2	,,,,,	re – Calculated	= Residual	Reference		,	re – Calculated	. , . , . ,	Reference
Gas Phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ =$	475.97 985.50	- 605.83 476.24 988.00	- 0.27 - 2.50	69STU/WES 69STU/WES	Gas Phase $\Delta_t H^\circ = C_\rho^\circ =$	-301.20	-300.81 132.92	-0.39	85MAJ/SVO
$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$		- 1971.32 - 18.08 7.29			Liquid Pha $\Delta_t H^\circ = C_p^\circ =$	se 356.60	-355.20 203.04	- 1.40	65CHA/ROS
Liquid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	se	-738.05 662.32 742.62			$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$		251.57 663.08 157.50 63.54		
$\Delta_{f}S^{\circ} = \\ \Delta_{f}G^{\circ} = \\ \ln K_{f} = $		-2216.69 -77.14 31.12			(2×C-(I	(C) + (1	oamyl alcohol ×C-(H) ₂ (C) ₂) iary)) + (1 × C-	+ (1 × C-(H)(((H) ₂ (O)(C)) +	C ₃ H ₁₂ C C) ₃) + (1 × O-(H)(C))
Solid Phase $\Delta_t H^\circ = C_p^\circ =$		-808.78 513.18				Literatui	re – Calculated	= Residual	Reference
$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$		524.22 - 2435.09 - 82.76 33.38			Gas Phase $\Delta_t H^\circ = C_r^\circ =$	- 300.80	- 303.07 132.92	2.27	85MAJ/SVO
(2×C-(I	H) ₃ (C)) + (1 H) ₂ (O)(C))	Isobutyl alcohol × C-(H)(C) ₃) - + (1 × O-(H)(C) re – Calculated	+ (2×-CH ₃ co ())	C ₄ H ₁₀ O orr (tertiary))+	Liquid Pha $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = $	se - 356.40 209.50	-357.38 203.04 251.57 -663.08	0.98 6.46	65CHA/ROS 45ZHD
Gas Phase $\Delta_t H^\circ =$	- 283.80	- 282.44	-1.36	66WAD2	$\Delta_{f}G^{\circ} = \\ \ln K_{f} = $		- 159.68 64.42		
C _p =		110.03			$(5 \times C_B - ($	$H)(C_B)_2) +$	zyl alcohol; Ph (1×C _B -(C)(C _E		C ₇ H ₈ O H)(C))+
Liquid Pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$	-334.70 181.00 214.51	-331.65 172.62 219.19	-3.05 8.38 -4.68	60SKI/SNE 60SKI/SNE 68COU/LEE	(1×C-(I	H) ₂ (O)(C _B)) Literatur	e – Calculated	= Residual	Reference
$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$		-559.15 -164.94 66.54			Gas Phase Δ _I H° =	- 100.42	-100.40	-0.02	26MAT
					Liquid Phas $\Delta_t H^\circ = C_p^\circ =$		- 160.71 214.62	0.00 1.32	54PAR/MAN 75NIC/WAD

TABLE 15. Alcohols (69) - Continued

2-Ethyl-1-hexanol	C ₈ H ₁₈ O
$(2 \times C - (H)_3(C)) + (4 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)_3) +$	

 $(2 \times C - (H)_3(C)) + (4 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)_3) + (1 \times C - (H)_2(O)(C)) + (1 \times O - (H)(C))$

	Literature - Calculated = Residual			Reference				
Gas Phase								
$\Delta_t H^\circ =$		- 360.44						
$C_p^{\circ} =$		201.59						
Liquid Phase $\Delta_t H^\circ = -$ $C_p^\circ = $ $S^\circ = $ $\Delta_t S^\circ = $	432.80	-430.21 294.30 348.71 -974.87	-2.59	60TJE				

2-Propanol; Isopropyl alcohol C_3H_8O $(2 \times C_-(H)_5(C)) + (1 \times C_-(H)(O)(C)_2 \text{ (alcohols, peroxides))} + (1 \times O_-(H)(C)) + (2 \times -CH_3 \text{ corr (tertiary)}), <math>\sigma = 18$

	Literature - Calculated = Residual			Reference			
Gas Phase							
$\Delta_{\rm f}H^{\circ} =$	-272.80	- 274.47	1.67	66WAD2			
$C_p^{\circ} =$	88.74	89.58	-0.84	69STU/WES			
S° =	309.91	309.06	0.85	69STU/WES			
$\Delta_f S^{\circ} =$		- 332.97					
$\Delta_f G^\circ =$		-175.20					
ln <i>K</i> ₁ =		70.67					
Liquid Ph	ase						
$\Delta_t H^{\circ} =$	- 318.10	-318.68	0.58	61SNE/SKI			
$C_p^{\circ} =$	154.43	167.43	-13.00	63AND/COU2			
S° =	180.58	180.66	-0.08	63AND/COU2			
$\Delta_{\rm p} S^{\circ} =$		-461.37					
$\Delta_{\rm f}G^{\circ} =$		- 181.12					
$lnK_f =$		73.06					

2-Butanol; sec-Butyl alcohol $(2\times C-(H)_3(C)) + (1\times C-(H)_2(C)_2) + \\ (1\times C-(H)(O)(C)_2 \ (alcohols,peroxides)) + (1\times O-(H)(C)) + \\ (1\times -CH_3 \ corr \ (tertiary)), \ \sigma = 9, \ \eta = 2$

	Literatu	Reference					
Gas Phase							
$\Delta_l H^\circ =$	- 292.70	- 292.84	0.14	91STE/CHI			
$C_p^{\circ} =$	113.30	112.47	0.83	69STU/WES			
S° =	359.03	359.74	-0.71	69STU/WES			
$\Delta_f S^\circ =$		-418.59					
$\Delta_f G^{\circ} =$		-168.04					
$lnK_f =$		67.78					

2-Butanol; sec-Butyl alcohol	C ₄ H ₁₉ O
$(2 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) +$	
$(1 \times C - (H)(O)(C)_2$ (alcohols, peroxides)) + $(1 \times O - (H)(C))$ +	
$(1 \times -CH_3 \text{ corr (tertiary)}), \sigma = 9, \eta = 2$	

	Literatu	Reference				
Liquid Phase						
$\Delta_{\rm f} H^{\circ} =$	-342.60	-342.23	0.37	91STE/CHI		
$C_p^{\circ} =$	197.40	197.85	0.45	71AND/CON		
S° =	213.10	213.04	0.06	71AND/CON		
$\Delta_f S^\circ =$		-565.30				
$\Delta_{\mathbf{f}}G^{\circ} =$		- 173.69				
$lnK_f =$		70.06				

2-Pentanol	$C_5H_{12}O$
$(2 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)_2) +$	
$(1 \times C - (H)(O)(C)_2$ (alcohols, peroxides)) + $(1 \times O - (H)(C))$ +	
$(1 \times -CH_3 \text{ corr (tertiary)}), \sigma = 9, \eta = 2$	

Literature – Calculated = Residual			Reference	
- 312.00	-313.47	1.47	85MAJ/SVO	
	135.36			
	398.90			
	-515.75			
	- 159.98			
	64.42			
e 366.20	- 367.96	1.76	74SAC/PES	
	-367.96 228.27	1.76	74SAC/PES	
		1.76	74SAC/PES	
	228.27	1.76	74SAC/PES	
	228.27 245.42	1.76	74SAC/PES	
		- 312.00 - 313.47 135.36 398.90 - 515.75 - 159.98	-312.00 -313.47 1.47 135.36 398.90 -515.75 -159.98	

-Pentanol	C5H12O
$(2 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)_2) +$	
$(1 \times C - (H)(O)(C)_2$ (alcohols, peroxides)) +	
$(1 \times O - (H)(C)), \sigma = 3$	

	Literature – Calculated = Residual			Reference	
Gas Phase					
$\Delta_t H^{\circ} = -$	314.60	-311.21	- 3.39	85MAJ/SVO	
$C_p^{\circ} =$		135.36			
S° =		402.28			
$\Delta_f S^\circ =$		-512.37		*	
$\Delta_t G^{\circ} =$		-158.45			
$lnK_f =$		63.92		·	
Liquid Phase					
$\Delta_f H^\circ = -$	368.60	-365.78	-2.82	74SAC/PES	
$C_{p}^{\circ} =$	240.00	228.27	11.73	76CON/GIN	
S° =		245.42			
$\Delta_f S^\circ =$		-669.23			
$\Delta_f G^\circ =$		-166.25			
$lnK_f =$		67.06			

TABLE 15. Alcohols (69) - Continued

2-Hexanol $(2 \times C - (H)_3(C)) + (3 \times C - (H)_2(C)_2) + (1 \times C - (H)(O)(C)_2 \text{ (alcohols, peroxides)}) + (1 \times O - (H)(C)) + (1 \times -CH_3 \text{ corr (tertiary)}), \sigma = 9, \eta = 2$	H ₁₄ O 4-Methyl-2-pentanol (Continued) $C_6H_{14}O$ $(3 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) +$ $(1 \times C - (H)(O)(C)_2 \text{ (alcohols, peroxides)}) + (1 \times O - (H)(C)) +$ $(1 \times C - (H)(C)_3) + (3 \times - CH_3 \text{ corr (tertiary)}), \sigma = 27, η = 2$
Literature - Calculated = Residual Reference	Literature – Calculated = Residual Reference
Gas Phase $ \Delta_{f}H^{\circ} = -329.90 -334.10 4.20 85MAJ/SV $ $ C_{p}^{\circ} = 158.25 $ $ S^{\circ} = 438.06 $ $ \Delta_{f}S^{\circ} = -612.90 $ $ \Delta_{f}G^{\circ} = -151.36 $ $ \ln K_{f} = 61.06 $	Liquid Phase O $\Delta_t H^\circ = -394.70$ - 398.97 4.27 74SAC/PES $C_p^\circ = 255.71$ $S^\circ = 272.45$ $\Delta_t S^\circ = -778.51$ $\Delta_t G^\circ = -166.86$ $\ln K_t = 67.31$
Liquid Phase $\Delta_t H^\circ = -388.40 -393.69 \qquad 5.29 \qquad 74SAC/PE$ $C_\rho^\circ = \qquad 258.69$ $S^\circ = \qquad 277.80$ $\Delta_t S^\circ = \qquad -773.16$ $\Delta_t G^\circ = \qquad -163.17$ $\ln K_t = \qquad 65.82$	S 2-Methyl-3-pentanol $C_6H_{14}O$ $(3\times C-(H)_3(C))+(1\times C-(H)_2(C)_2)+(1\times C-(H)(C)_3)+$ $(1\times O-(H)(C))+(1\times C-(H)(O)(C)_2 \text{ (alcohols, peroxides)})+$ $(2\times -CH_3 \text{ corr (tertiary)}), \sigma = 27, \eta = 2$ Literature – Calculated = Residual Reference
$(2 \times C - (H)_3(C)) + (3 \times C - (H)_2(C)_2) + (1 \times O - (H)(C)) + (1 \times C - (H)(O)(C)_2 \text{ (alcohols, peroxides)}), \ \sigma = 9, \ \eta = 2$	H ₁₄ O Gas Phase $\Delta_t H^\circ = -338.53$ $C_p^\circ = 158.28$ $S_p^\circ = 424.33$
Literature - Calculated = Residual Reference	$\Delta_t G^{\circ} = -151.70$
Gas Phase $ \Delta_{t}H^{\circ} = -331.84 $ $ C_{p}^{\circ} = 158.25 $ $ S^{\circ}(J/\text{mol·K}) = 438.06 $ $ \Delta_{t}S^{\circ}(J/\text{mol·K}) = -612.90 $ $ \Delta_{t}G^{\circ} = -151.36 $	$\ln K_{\rm f} =$ 61.20 Liquid Phase $\Delta_t H^{\circ} = -396.40 - 396.79 0.39$ 74SAC/PES $C_{\rm f}^{\circ} =$ 255.71 $S^{\circ} =$ 272.45
Liquid Phase $\Delta_{i}H^{\circ} = -392.40 -391.51 -0.89 85MAJ/SV$	$\Delta_{f}S^{\circ} = -778.51$ $\Delta_{f}G^{\circ} = -164.68$ $\ln K_{f} = 66.43$
$C_p^{\circ} = 286.00$ 258.69 27.31 76CON/G $S^{\circ} = 277.80$ $\Delta_t S^{\circ} = -773.16$ $\Delta_t G^{\circ} = -160.99$ $\ln K_t = 64.94$	2-Methyl-2-propanol; tert-Butyl alcohol $(3 \times C - (H)_3(C)) + (1 \times C - (O)(C)_3 \text{ (alcohols,peroxides)}) + (1 \times O - (H)(C)) + (3 \times - CH_3 \text{ corr (quaternary)}), \sigma = 81$
	Literature - Calculated = Residual Reference
$(3 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) +$ $(1 \times C - (H)(O)(C)_2 \text{ (alcohols, peroxides)}) + (1 \times O - (H)(C)) +$ $(1 \times C - (H)(C)_3) + (3 \times - CH_3 \text{ corr (tertiary)}), \sigma = 27, \eta = 2$ $\text{Literature} - \text{Calculated} = \text{Residual} \qquad \text{Reference}$	Gas Phase $\Delta_t H^\circ = -312.60 -313.29 0.69 66WAD2$ $C_c^\circ = 113.39 111.08 2.31 69STU/WES$ $S^\circ = 326.27 322.32 3.95 69STU/WES$
Gas Phase $\Delta_{t}H^{\circ} = -340.79$ $C_{p}^{\circ} = 158.28$ $S^{\circ}(J/\text{mol-K}) = 424.33$ $\Delta_{t}S^{\circ}(J/\text{mol-K}) = -626.63$ $\Delta_{t}G^{\circ}(J/\text{mol-K}) = -153.96$ $\ln K_{t} = 62.11$	$\Delta_{t}S^{\circ} = -456.01$ $\Delta_{t}G^{\circ} = -177.33$ $\ln K_{t} = 71.53$

TABLE 15. Alcohols (69) — Continue	ohols (69) - Continue	d
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(3×C-($(H)_3(C))+(1$	ert-Butyl alcol ×C-(O)(C) ₃ (×-CH ₃ corr (c	alcohols,perox	ides))+
	Literatur	re – Calculated	= Residual	Reference
Liquid Ph	ase			
$\Delta_{\rm f}H^{\circ} =$	-359.20	-358.63	-0.57	60SKI/SNE
	219.66	219.66	0.00	63OET
S° =	171.31	171.31	0.00	63OET
$\Delta_t S^{\circ} =$		-607.03		
$\Delta_{\rm f}G^{\circ} =$		- 177.65		
$lnK_f =$		71.66		
Solid Pha	se			
$\Delta_{\rm f}H^{\circ} =$	- 365.90	-365.18	-0.72	63OET
$C_p^{\circ} =$	146.11	146.12	-0.01	63OET
s° =		183.92	-13.05	63OET
$\Delta_f S^\circ =$		-594.42		
$\Delta_i G^{\circ} =$		- 187.95		
$lnK_f =$		75.82		

2-Methyl-2-butanol C₃H₁₂O

 $(3 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (O)(C)_3 \text{ (alcohols, peroxides)}) + (1 \times O - (H)(C)) +$

 $(2 \times -CH_3 \text{ corr (quaternary)}), \sigma = 27$

	Literatu	Literature – Calculated ≈ Residual					
Gas Phase							
$\Delta_f H^\circ =$	-329.40	-329.36	-0.04	85MAJ/SVO			
$C_p^{\circ} =$	131.67	133.97	-2.30	69STU/WES			
s° =	366.85	370.62	-3.77	69STU/WES			
$\Delta_f S^\circ =$		- 544.03					
$\Delta_f G^{\circ} =$		- 167.16					
$lnK_f =$		67.43					
Liquid Ph	ase						
$\Delta_t H^\circ =$	-379.50	-379.97	0.47	65CHA/ROS			
$C_p^{\circ} =$	247.30	250.08	-2.78	83DAP/DEL			
S° =		203.69					
$\Delta_f S^\circ =$		~710.96					
$\Delta_t G^{\circ} =$		- 168.00					
$lnK_f =$		67.77					

$$\label{eq:continuous} \begin{split} & \textbf{Triphenylmethanol; Triphenylcarbinol} & C_{19}H_{16}O\\ & (15\times C_B-(H)(C_B)_2) + (3\times C_B-(C)(C_B)_2) + (1\times O-(H)(C)) + \\ & (1\times C-(O)(C_B)_3) \end{split}$$

	Literature	e – Calculated	Reference	
Solid Phase	•			
$\Delta_i H^\circ =$	-2.51	0.45	-2.96	54PAR/MAN
$C_p^{\circ} =$	318.80	318.91	-0.11	31SMI/AND

1,2-Ethane (2×C-(C₂H ₆ O			
	Literatu	re – Calculated	= Residual	Reference
Gas Phase				
$\Delta_t H^\circ =$	-387.50	- 384.46	-3.04	29PAR/KEL
$C_p^{\circ} =$	97.07	76.98	20.09	69STU/WES
S° =	323.55	324.10	-0.55	69STU/WES
Δ ₆ S° ==		- 284.14		
$\Delta_{\rm f}G^{\circ} =$		- 299.74		
$lnK_f =$		120.91		
Liquid Pha	ise			
$\Delta_t H^\circ =$	-455.30	-454.60	-0.70	29PAR/KEL
$C_p^{\circ} =$	149.30	156.56	- 7.26	79STE/TAM
S° =	166.90	152.96	13.94	25PAR/KEL
$\Delta_f S^\circ =$		-455.28		
$\Delta_l G^{\circ} =$		- 318.86		
$lnK_f =$		128.63		

1,2-Propanediol; Propylene glycol

 $C_3H_8O_2$

 $(1 \times C - (H)_3(C)) + (2 \times O - (H)(C)) +$

 $(1 \times C - (H)(O)(C)_2$ (alcohols, peroxides)) + $(1 \times C - (H)_2(O)(C))$ +

(1×-CH₃ corr (tertiary))

	Literature – Calculated = Residual			idual Reference	
Gas Phas	e				
$\Delta_f H^\circ =$	- 421.30	-422.18	0.88	72GAR/HUS	
$C_p^{\circ} =$		102.34			
Liquid Ph		- 496.19	10.49	72GAR/HUS	
$\Delta_i H^\circ =$				1200111100	
$C_p^o =$	188.10	209.23	-21.13	85WIL/CHA	
•		209.23 173.84	-21.13		
$C_p^o =$			-21.13		
$C_p^{\circ} = S^{\circ} =$		173.84	-21.13		

1,3-Propanediol; Trimethylene glycol

)

Reference

C₃H₈O₂

 $(1 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(O)(C)) + (2 \times O - (H)(C))$ Literature – Calculated = Residual Reference

Gas Phase $\Delta_t H^\circ = C_p^\circ =$	- 392.10	- 405.09 99.87	12.99	72GAR/HUS
Liquid Phas	se			
$\Delta_t H^\circ =$	- 480.80	-480.33	-0.47	89KNA/SAB
$C_p^{\circ} =$		186.98		
$C_p^{\circ} = S^{\circ} = 0$		186.98 185.34		
S° =		185.34		

TABLE 15. Alcohols (69) - Continued

1,2,3-Propanetriol; Glycerol	C ₃ H ₈ O ₃
$(2 \times C - (H)_2(O)(C)) + (1 \times C - (H)(O)(C)_2$ (alcoho	ls,peroxides))+
$(3\times O-(H)(C))$	

	Literature – Calculated = Residual			Residual Reference	
Gas Phase $\Delta_t H^\circ =$	e - 577.90	- 569.89	-8.01	88BAS/NIL	
$C_p^{\circ} =$	377,50	115.10	0.01	002110,1112	
7 '' 1 Di					
Liquid Ph		673 70	A 10	III/N 2 A G/S	
$\Delta_i H^o =$	- 669.60	-673.70 251.03	4.10 - 32.03	88BAS/NIL	
$\Delta_i H^\circ = C_p^\circ =$	- 669.60 219.00	251.03	-32.03	88BAS/NIL	
$\Delta_{i}H^{\circ} = C_{p}^{\circ} = S^{\circ} =$	- 669.60	251.03 167.02			
$\Delta_i H^\circ = C_p^\circ =$	- 669.60 219.00	251.03	-32.03	88BAS/NIL	

1,2-Butanediol	C ₄ H ₁₀ O ₂
$(1 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(O)(C)) +$	
$(1 \times C - (H)(O)(C)_2$ (alcohols, peroxides)) + $(2 \times O - (H)(C))$	

	Literatui	re – Calculated –––––	= Residual	Reference
Gas Phase				
$\Delta_i H^\circ =$		- 440.55		
$C_p^{\circ} =$		125.23		
Liquid Ph $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	ase - 523.60	- 519.74 239.65 206.22 - 674.64 - 318.60 128.52	-3.86	37MOU/DOD

$\begin{array}{ll} \textbf{1,3-Butanediol} & C_4H_{10}O_2 \\ (1\times C-(H)_3(C)) + (1\times -CH_3 \ corr \ (tertiary)) + (1\times C-(H)_2(C)_2) + \\ (2\times O-(H)(C)) + (1\times C-(H)_2(O)(C)) + \\ (1\times C-(H)(O)(C)_2 \ (alcohols,peroxides)) \end{array}$

Literatu	re – Calculated	= Residual	Reference
Gas Phase			
$\Delta_t H^{\circ} = -433.20$	-442.81	9.61	72GAR/HUS
$C_p^{\circ} =$	125.23		
Liquid Phase $\Delta_t H^\circ = -501.00$ $C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t = S^\circ = S$	-521.92 239.65 206.22 -674.64 -320.78 129.40	20.92	72GAR/HUS

1,4-Butanediol	$C_4H_{10}O_2$
$(2 \times O - (H)(C)) + (2 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(O)(C))$	

	Literatu	re – Calculated	= Residual	Reference
Gas Phase	e			
$\Delta_{\rm f}H^{\circ} =$	-426.70	-425.72	-0.98	72GAR/HUS
$C_p^{\circ} =$		122.76		
Liquid Ph				*
Liquid Ph $\Delta_t H^\circ =$	ase - 505.30	- 506.06	0.76	89KNA/SAB
$\Delta_{\rm f} H^{\circ} = C_{\rm p}^{\circ} =$		- 506.06 217.40	0.76 - 17.30	89KNA/SAB 84VAS/PET
$\Delta_t H^\circ = C_p^\circ = S^\circ = S$	-505.30			
$\Delta_{\rm f} H^{\circ} = C_{\rm p}^{\circ} =$	-505.30 200.10	217.40	-17.30	84VAS/PET
$\Delta_t H^\circ = C_p^\circ = S^\circ = S$	-505.30 200.10	217.40 217.72	-17.30	84VAS/PET

2,3-Butanediol $C_4H_{10}O_2$ $(2\times C-(H)_3(C))+(2\times C-(H)(O)(C)_2$ (alcohols,peroxides))+

 $(2\times O-(H)(C))+(2\times -CH_3 \text{ corr (tertiary)})$

Gas Phas		re – Calculated	l = Residual	Reference
$ \frac{\Delta_{f}H^{\circ} =}{C_{p}^{\circ} =} $	-482.30	-459.90 127.70	- 22.40	46KNO/SCH
Liquid Ph	ase	:		
$\Delta_{\rm f} H^{\circ} =$	-541.50	~537.78	-3.72	37MOU/DOD
$C_p^{\circ} =$	213.00	261.90	48.90	36KHO/KAL
S° =		194.72		
$\Delta_f S^\circ =$		-686.14		
$\Delta_f G^\circ =$		-333.21		
$lnK_f =$		134.41		

$\begin{array}{ll} \textbf{2-Methyl-1,2-propanediol} & \textbf{C_4H_{10}O_2} \\ (2\times O-(H)(C)) + (2\times C-(H)_3(C)) + (2\times -CH_3 \text{ corr (quaternary)}) + \\ (1\times C-(O)(C)_3 \text{ (alcohols,peroxides)}) + (1\times C-(H)_2(O)(C)) \end{array}$

Gas Phase	Literatur	e – Calculated	= Residual	Reference
$\Delta_i H^\circ =$		-458.70		
$C_p^{\circ} =$		123.84		
Liquid Phase $\Delta_t H^\circ = -1$	539.70	- 533.93	- 5.77	37MOU/DOD
$C_p^{\circ} = S^{\circ} = S$	339.70	261.46 164.49	-3.77	3/MOO/DOD
$\Delta_{f}S^{\circ} =$		-716.37		
$\Delta_t G^\circ = \ln K_t =$		-320.34 129.22		

TABLE	15.	Alcohols	(69)	_	Continued
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(2,70 (1		rythritol < C-(H) ₂ (O)(C alcohols,peroxi		C ₄ H ₁₀ O ₄	Pentaery	thritol (Co	d)-1,3-propaned atinued) \times C-(C) ₄) + (4	•	C ₅ H ₁₂ O ₅
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	-775.20	-755.32 153.22	- 19.88	50NIT/SEK	Liquid pha $ \Delta_t H^\circ = C_p^\circ = S^\circ = $	se	891.21 323.36 207.27		
Liquid pha Δ _ε H° =	se -887.00	- 892.80	5.80	52PAR/MAN	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		- 1014.94 - 588.61 237.44	···	
$C_p^o = S^o = S^o = \Delta_t S^o = InK_t = InK_t$		345.50 181.08 - 904.82 - 623.03 251.33			Solid phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \Delta_t G^\circ = S^\circ = S^\circ$	- 920.60 190.41 198.07	-918.17 121.05 180.21 -1042.00 -607.50	2.43 69.36 17.86	54MED/THO 59WES 59WES
Solid phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = $	- 910.40 170.70 177.80	- 922.80 170.38 177.84 - 908.06 - 652.06	12.40 0.32 0.04	46PAR/WES 32SPA/THO 26PAR/AND	1,6-Hexane		245.06 2×C-(H) ₂ (O)(C))+(2×O-(C ₆ H ₁₄ O ₂ H)(C))
InK _f =		263.04				Literatu	re – Calculated	= Residual	Reference
1,5-Pentano (2×O-()	H)(C))+(3:	× C-(H) ₂ (C) ₂)	+ (2×C~(H) ₂ (C ₅ II ₁₂ O ₂ O)(C))	Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 459.40	466.98 168.54	7.58	91STE/CHI
		e - Calculated	= Residual	Reference	C_p –		100.54		
Gas phase $\Delta_t H^\circ = C_p^\circ -$	- 448.99	- 446.35 145.65	= Residual - 2.64	Reference 72GAR/HUS	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = S^\circ$	se - 562.30	-557.52 278.24 282.48	- 4.78	91STE/CHI
$\Delta_t H^{\circ} = C_p^{\circ} -$ Liquid pha $\Delta_t H^{\circ} =$	~448.99	-446.35 145.65 -531.79			Liquid phas $\Delta_t H^\circ = C_p^\circ =$		-557.52 278.24	-4.78	91STE/CHI
$\Delta_{t}H^{\circ} = C_{p}^{\circ} -$ Liquid pha	~448.99	- 446.35 145.65	-2.64	72GAR/HUS	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ - \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \Delta_t H^\circ = C_\rho^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t$	- 562.30	- 557.52 278.24 282.48 - 871.00 - 297.83 120.14 - 582.96 190.02 198.74 - 954,74	- 4.78 - 0.90 13.21	91STE/CHI 91STE/CHI 91STE/CHI
$\Delta_t H^\circ = C_p^\circ -$ Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_f =$ 2,2'-Bis(hy)	448.99 sse 531.49 droxymethyl	- 446.35 145.65 - 531.79 247.82 250.10 - 767.07 - 303.09	-2.64 0.30	72GAR/HUS 72GAR/HUS C5H12O4	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ - \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f = \frac{1}{2}$ Solid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = S^\circ = \frac{1}{2}$	-562.30 -583.86	-557.52 278.24 282.48 -871.00 -297.83 120.14 -582.96 190.02 198.74	- 0.90	91STE/CHI
$\Delta_t H^\circ = C_p^\circ -$ Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t =$ 2,2'-Bis(hy)	- 448.99 ise - 531.49 droxymethyl thritol H)(C)) + (12	- 446.35 145.65 - 531.79 247.82 250.10 - 767.07 - 303.09 122.26	-2.64 0.30 liol; × C-(H) ₂ (O)(0	72GAR/HUS 72GAR/HUS C5H12O4	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{\Delta_t G^\circ}{S^\circ} = \frac{\Delta_t G^\circ}{S^\circ} = \frac{\Delta_t S^\circ}{S^\circ} = \Delta_t S^\circ$	- 562.30	- 557.52 278.24 282.48 - 871.00 - 297.83 120.14 - 582.96 190.02 198.74 - 954.74 - 298.30	-0.90 13.21	91STE/CHI 91STE/CHI CLeH22O2
$\Delta_t H^\circ = C_p^\circ -$ Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t =$ 2,2'-Bis(hy)	- 448.99 ise - 531.49 droxymethyl thritol H)(C)) + (12	- 446.35 145.65 - 531.79 247.82 250.10 - 767.07 - 303.09 122.26 × C-(C) ₄) + (4:	-2.64 0.30 liol; × C-(H) ₂ (O)(0	72GAR/HUS 72GAR/HUS C5H12O4	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{\Delta_t G^\circ}{S^\circ} = \frac{\Delta_t G^\circ}{S^\circ} = \frac{\Delta_t S^\circ}{S^\circ} = \Delta_t S^\circ$	- 562.30 - 583.86 203.60 edial H ₂ (C) ₂) + (2	- 557.52 278.24 282.48 - 871.00 - 297.83 120.14 - 582.96 190.02 198.74 - 954.74 - 298.30 120.33	-0.90 13.21 +(2×C-(H)₂(91STE/CHI 91STE/CHI CLeH22O2

TABLE 15. Alcohols (69) - Continued

1,10-Decanediol (Continued) $(8 \times C-(H)_2(C)_2) + (2 \times O-(H)(C)) + (2 \times C-(H)_2(C)_2) + (2 \times O-(H)(C)_2) + (2 \times C-(H)_2(C)_2) + (2 \times $	$C_{10}H_{22}O_2$ (O)(C))	(1×O-(1	H)(C)) + (1	xyl alcohol (Co ×C-(H)(O)(C) 1×Cyclohexano	2 (alcohols,pe	
Literature - Calculated = Residual	Reference	(0.1.0 (.	.2)2(0)2) . (1 / Cyclonoman	(500) 150), 0	•
			Literatu	re – Calculated	= Residual	Reference
Liquid phase						
$\Delta_t H^\circ = -660.44$		Liquid pha	se			
$C_p^{\circ} = 0.000$ 399.92		$\Delta_{\rm f}H^{\circ} =$	-348.60	-349.81	1.21	62RAB/TEL
$S^{\circ} = 412.00$		$C_p^{\circ} =$	213.59	220.36	-6.77	68ADA/SUG
$\Delta_{\rm f} S^{\circ} = -1286.72$		<i>s</i> ° =	203.87	201.06	2.81	68ADA/SUG
$\Delta_{\rm f}G^{\circ} = -276.80$		$\Delta_f S^\circ =$		- 719.33		
$\ln K_{\rm f} = 111.66$		$\Delta_{\mathbf{f}}G^{\circ} =$		- 135.34		
		$lnK_f =$		54.60		
Solid phase						
$\Delta_t H^{\circ} = -693.50 -700.60$ 7.10	62PAR/MOS					
$C_{P}^{\circ} = 277.70$		Cyclohepta	nol; Cycloh	eptyl alcohol		C7H14C
$S^{\circ} = 290.78$		(1×O-()	H)(C)) + (1	×C-(H)(O)(C)	2 (alcohols, pe	roxides))+
$\Delta_{\mathbf{f}}S^{\circ} = -1407.94$				1 × Cycloheptar		,,,
$\Delta_{\rm f}G^{\circ} = -280.82$		•		•	•	
$lnK_f = 113.28$			Literatu	re – Calculated	= Residual	Reference
		Gas phase		202.05		
Cyclopentanol; Cyclopentyl alcohol	C ₅ H ₁₀ O	$\Delta_{\rm f}H^{\circ} =$		- 282.87		
$(1 \times O - (H)(C)) + (1 \times C - (H)(O)(C)_2$ (alcohols, pe	eroxides))+	$C_p^{\circ} =$		138.32		
$(4 \times C - (H)_2(C)_2) + (1 \times Cyclopentane (sub) rsc)$						
Literature - Calculated = Residual	Reference	Liquid pha $\Delta_t H^\circ =$	se	240.00		
		$C_p^{\circ} =$	250.20	-349.98 244.80	5.40	72ADA/SUG
Gas phase		$S^{\circ} =$	241.63	224.23	17.40	•
Gas phase $\Delta_t H^\circ = -242.60 -248.40$ 5.80	62SEL/SUN	$\Delta_6 S^\circ =$	241.03		17.40	72ADA/SUG
-	023EL/3UN	$\Delta_{f}S = \Delta_{f}G^{\circ} =$		- 832.47		
$C_p^{\circ} = 101.81$		$\ln K_{\rm f} =$		- 101.78 41.06		
Liquid phase						
$\Delta_t H^{\circ} = -300.00 -298.43 -1.57$	62SEL/SUN	1-Adamant	anol			C10H16C
$C_p^{\circ} = 184.10 192.83 -8.73$	56PAR/KEN			\times C-(H) ₂ (C) ₂)	± (1 ∨ Adama	
$S^{\circ} = 206.30 200.23 6.07$	56PAR/KEN			phols, peroxides		
$\Delta_{\rm f} S^{\circ} = -583.85$	Jorrhynder	(170 ()(C)3 (alce	mois,peroxides	,, 1 (1 / 0 (11)(C))
$\Delta_f G^\circ = -124.36$			Literatus	re – Calculated	- Decidual	Reference
$\ln K_{\rm f} = 50.16$			Literatur		- Acsiduai	
		Gan mhana				
		Gas phase $\Delta_t H^\circ =$	-310.90	-306.26	- 4.64	78ARO/STE
Cyclohexanol; Cyclohexyl alcohol	C ₆ H ₁₂ O					
$(1 \times O-(H)(C)) + (1 \times C-(H)(O)(C)_2$ (alcohols, pe	eroxides)) +					
$(5 \times C - (H)_2(C)_2) + (1 \times Cyclohexane (sub) rsc), or$	r = 1	Solid phase	:			
		$\Delta_{f}H^{\circ} =$	-397.50	-403.13	5.63	78ARO/STE
Literature – Calculated = Residual	Reference					
		2-Adamant				C10H16O
Gas phase			, . ,	\times C-(H) ₂ (C) ₂)·	•	ntane rsc)+
$\Delta_{\ell}H^{\circ} = -286.20 -288.97$ 2.77	66WAD2	(1×C-(F	I) ₂ (O)(C)) -	+ (1 × O-(H)(C))	
$C_p^{\circ} = 127.24 129.75 -2.51$	69STU/WES					
$S^{\circ} = 360.04 \qquad 358.22 \qquad 1.82$	69STU/WES		Literatur	re – Calculated :	= Residual	Reference
$\Delta_{\mathbf{f}}S^{\circ} = -562.17$						
$\Delta_t G^{\circ} = -121.36$						
$\ln K_{\rm f} = 48.96$		Gas phase				
		$\Delta_i H^\circ =$	-299.20	-306.20	7.00	78ARO/STE
					 	
		Solid phase $\Delta_t H^\circ =$	- 38 7.9 0	-400.45	12.55	78ARO/STE

	Literatur	e - Calculated	= Residual	Reference					
						Literatu	re – Calculated	= Residual	Reference
as phase	14 ,								
$\Lambda_t H^{\circ} =$	- 96.40	- 96.00	-0.40	60AND/BID	Gas phase				
$C_{p}^{\circ} =$	103.55	102.07	1.48	69STU/WES	$\Delta_{\rm f}H^{\circ} =$	-132.30	- 129.06	- 3.24	60AND/BID
S° =	315.60	313.57	2.03	69STU/WES	$C_p^{\circ} =$	122.47	124.65	-2.18	69STU/WES
Δ _t S° =	, 515.00	-215.11	2.00		S° =	356.77	353.60	3.17	69STU/WE
					Δ _i S° =	550.77	-311.39	5.17	070107112
$G^{\circ} =$		-31.87		*					
$\ln K_{\rm f} =$		12.85			$\Delta_f G^\circ = \ln K_f =$		- 36,22 14.61		
quid phas	re.								
l _l H° =	- 153.86	- 156.56	2.70	63AND/COU	Liquid pha		40- :-		·- ·
$C_p^{\circ} =$		197.75			$\Delta_l H^o =$	- 194.00	- 193,17	- 0.83	60AND/BII
S° =		177.65			$C_p^{\circ} =$	224.93	221.65	3.28	67AND/CO
Δ _f S° =		-351.02			S° =	212.59	212.58	0.01	67AND/CO
$_{i}G^{\circ} =$		-51.90			$\Delta_f S^\circ =$		-452.41		
$\ln K_{\rm f} =$		20.94			$\Delta_f G^\circ =$		-58.29		
					$\ln K_{\rm f} =$		23.51		
olid phase	;								
MH° =	- 165.10	- 165.60	0.50	60AND/BID					
$C_p^{\circ} =$	127.44	129.61	-2.17	63AND/COU	4-Mathylal	henol; p-Cre	eol		C ₇ 1
<i>S</i> ° =	144.01	143.96	0.05	63AND/COU	(1×C-($H_{3}(C) + (1$	\times O-(H)(C _B))	$+(4\times C_B-(H)$	$(C_B)_2$ +
Δ _f S° =		- 384.71			(1×C _B −	$(C)(C_B)_2)+c$	$(1 \times C_B - (O)C_B)$	$p_{2}, \sigma = 6$	
$_{if}G^{\circ} =$		- 50.90							
$lnK_f =$									To 0
-Methylph (1×C-(1		\times O-(H)(C _B))			Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 125.40 124.47	- 128.43 123.94	3.03 0.53	Reference 60AND/BID 69STU/WES
-Methylph (1×C-(l	$(C)(C_{B})_{2}$	sol	$+(1\times C_{\rm B}-(O))$	$(C_B)_2) +$	$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = 0$	-125.40	- 128.43 123.94 347.83 - 317.15 - 33.87	3.03	60AND/BID
-Methylph (1×C-(I (1×C _p -($(C)(C_{B})_{2}$	sol ×O-(H)(C _B)) (1×ortho corr)	$+(1\times C_{\rm B}-(O))$	$(C_B)_2) + ((C_D)_2), \sigma = 3$	$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = C_p^{\circ} = C_$	- 125.40 124.47	- 128.43 123.94 347.83 - 317.15	3.03 0.53	60AND/BID 69STU/WES
-Methylph $(1 \times C)$ -(1 $(1 \times C)$ -(1 Gas phase $\Delta_t H^\circ =$	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu 	sol × O-(H)(C _B)) (1 × ortho corr) re – Calculated – 127.17	$+ (1 \times C_{n} - (O))$ $= Residual$ -1.43	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid pha	125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87	3.03 0.53	60AND/BID 69STU/WES
-Methylph (1 × C-(I (1 × C _p -(H)3(C)) + (1 (C)(C _D)2) + Literatu	sol ×O-(H)(C _B)) (1×ortho corr) re – Calculated	+ (1 × C _D -(O)) = Residual	$(C_B)_2$ + $(C_D)_2$, $\sigma = 3$ Reference	$\Delta_t H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1}{2}$	125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87	3.03 0.53	60AND/BID
-Methylph $(1 \times C)$ -(1 $(1 \times C)$ -(1 Gas phase $\Delta_t H^\circ =$	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu 	sol × O-(H)(C _B)) (1 × ortho corr) re – Calculated – 127.17	$+ (1 \times C_{n} - (O))$ $= Residual$ -1.43	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid pha	125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66	3.03 0.53	60AND/BII 69STU/WES 69STU/WES
-Methylph $(1 \times C - (1 \times C_p - $	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33	sol ×O-(H)(C _B)) (1 × ortho corr) re - Calculated -127.17 130.34 351.10	+ $(1 \times C_{n}$ - (O) = Residual - 1.43 - 0.01	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference 60AND/BID 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid pha $\Delta_{t}H^{\circ} = \frac{1}{2}$	125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66	3.03 0.53 - 0.18	60AND/BII 69STU/WES 69STU/WES
Methylph $(1 \times C - (1 \times C_n - ($	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33	sol ×O-(H)(C _B)) (1 × onho corr) re - Calculated -127.17 130.34 351.10 -313.89	+ $(1 \times C_{n}$ - (O) = Residual - 1.43 - 0.01	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference 60AND/BID 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid pha $\Delta_{t}H^{\circ} = C_{p}^{\circ} - S^{\circ} = \frac{1}{2}$	125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58	3.03 0.53 - 0.18	60AND/BII 69STU/WES 69STU/WES
Methylph $(1 \times C - (1 \times C_n - ($	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33	Sol ×O-(H)(C _B)) (1 × ortho corr) re - Calculated -127.17 130.34 351.10 -313.89 -33.58	+ $(1 \times C_{n}$ - (O) = Residual - 1.43 - 0.01	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference 60AND/BID 69STU/WES	$\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = S_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid pha $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} - S^{\circ} = \Delta_{t}S^{\circ} = \frac{1}{2}$	125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41	3.03 0.53 - 0.18	60AND/BII 69STU/WE: 69STU/WE:
Methylph $(1 \times C - (1 \times C_n - ($	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33	sol ×O-(H)(C _B)) (1 × onho corr) re - Calculated -127.17 130.34 351.10 -313.89	+ $(1 \times C_{n}$ - (O) = Residual - 1.43 - 0.01	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference 60AND/BID 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid pha $\Delta_{t}H^{\circ} = C_{p}^{\circ} - S^{\circ} = \frac{1}{2}$	125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58	3.03 0.53 - 0.18	60AND/BII 69STU/WES 69STU/WES
-Methylph $(1 \times C_n - 1)$ is sphase $C_p^{\alpha} = C_p^{\alpha} = C_p^{\alpha} = C_p^{\alpha} = 1$ in $K_t = C_p^{\alpha}$ in $K_t = C_p^{\alpha}$	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	Sol ×O-(H)(C _B)) (1 × ortho corr) re - Calculated -127.17 130.34 351.10 -313.89 -33.58	+ $(1 \times C_{n}$ - (O) = Residual - 1.43 - 0.01	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference 60AND/BID 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid pha $\Delta_{t}H^{\circ} = C_{p}^{\circ} - S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \frac{1}{2}$	125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29	3.03 0.53 - 0.18	60AND/BIE 69STU/WES 69STU/WES
-Methylph $(1 \times C - (1 \times C_n - $	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	Sol ×O-(H)(C _B)) (1 × ortho corr) re - Calculated -127.17 130.34 351.10 -313.89 -33.58	+ $(1 \times C_{n}$ - (O) = Residual - 1.43 - 0.01	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference 60AND/BID 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid pha $\Delta_{t}H^{\circ} = C_{p}^{\circ} - S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \frac{1}{2}$	125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29	3.03 0.53 - 0.18	60AND/BII 69STU/WES 69STU/WES
-Methylph $(1 \times C_{-1})$ $(1 \times C_{-1})$ is sphase $\lambda_i H^\circ = C_\rho^\circ = S^\circ = \lambda_i G^\circ = \ln K_i = \lim_{\lambda_i \to 0} \lambda_i H^\circ = \lim_{\lambda_i \to 0} \lambda_i $	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	sol × O-(H)(C _B)) (1 × ortho corr) re - Calculated - 127.17 130.34 351.10 - 313.89 - 33.58 13.55	+ $(1 \times C_{n}$ - (O) = Residual - 1.43 - 0.01	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference 60AND/BID 69STU/WES	$\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Lambda_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid phase $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} - S^{\circ} = \Delta_{t}S^{\circ} = \Lambda_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Solid phase	125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29 23.51	3.03 0.53 -0.18	60AND/BIE 69STU/WES 69STU/WES
-Methylph $(1 \times C_n - 1)$ ias phase $\lambda_i H^\circ = C_\rho^\circ = S^\circ = \lambda_i G^\circ = \ln K_I = 1$ iquid pha	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	sol ×O-(H)(C _B)) (1×ortho corr) re - Calculated -127.17 130.34 351.10 -313.89 -33.58 13.55 -189.91 225.15	+ $(1 \times C_{n}$ - (O) = Residual - 1.43 - 0.01	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference 60AND/BID 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = InK_{t} = InK_{t} = InK_{t} = InK_{t}G^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = InK_{t} = InK_{t}G^{\circ} = InK_{t}G^{\circ$	125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29 23.51	3.03 0.53 -0.18	60AND/BIE 69STU/WES 69STU/WES 75NIC/WAI
-Methylph $(1 \times C - (1 \times C_n - $	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	sol ×O-(H)(C _B)) (1×ortho corr) re - Calculated -127.17 130.34 351.10 -313.89 -33.58 13.55 -189.91 225.15 212.58	+ $(1 \times C_{n}$ - (O) = Residual - 1.43 - 0.01	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference 60AND/BID 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = InK_{t} = InK_{t} = InK_{t} = InK_{t}G^{\circ} = InK_{t}G^{\circ}$	- 125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29 23.51	3.03 0.53 -0.18 0.61	60AND/BID 69STU/WES 69STU/WES 75NIC/WAI 60AND/BID 67AND/COI
-Methylph $(1 \times C_{-1})$ $(1 \times C_{n-1})$ Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S_0^\circ =$ $\Delta_t S_0^\circ =$ $\ln K_t =$ iquid pha $\Delta_t H^\circ =$ $S_0^\circ =$	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	sol ×O-(H)(C _B)) (1×ortho corr) re - Calculated -127.17 130.34 351.10 -313.89 -33.58 13.55 -189.91 225.15 212.58 -452.41	+ $(1 \times C_{n}$ - (O) = Residual - 1.43 - 0.01	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference 60AND/BID 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{S^{\circ}} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{1}{S^{\circ}} = $	125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29 23.51	3.03 0.53 -0.18	60AND/BID 69STU/WES
ias phase $C_p^{\rho} = S^{\circ} = \Delta_t S^{\circ} = \ln K_t = S^{\circ} = \Delta_t S^{\circ$	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	sol ×O-(H)(C _B)) (1×ortho corr) re - Calculated -127.17 130.34 351.10 -313.89 -33.58 13.55 -189.91 225.15 212.58 -452.41 -55.03	+ $(1 \times C_{n}$ - (O) = Residual - 1.43 - 0.01	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference 60AND/BID 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{C_{p}^{\circ} - S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ} - C_{p}^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = \frac{\Delta_{t}H^{\circ} - C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \frac{\Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \frac{\Delta_{t}S^{\circ} = C_{t}G^{\circ} $	- 125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29 23.51 - 204.97 153.67 172.40 - 492.59	3.03 0.53 -0.18 0.61	60AND/BID 69STU/WES 69STU/WES 75NIC/WAI 60AND/BID 67AND/COI
Methylph $(1 \times C_{-1})$ $(1 \times C_{n-1})$ $(1 \times C_{n-1}$	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	sol ×O-(H)(C _B)) (1×ortho corr) re - Calculated -127.17 130.34 351.10 -313.89 -33.58 13.55 -189.91 225.15 212.58 -452.41	+ $(1 \times C_{n}$ - (O) = Residual - 1.43 - 0.01	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference 60AND/BID 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} =$	- 125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29 23.51 - 204.97 153.67 172.40 - 492.59 - 58.11	3.03 0.53 -0.18 0.61	60AND/BID 69STU/WES 69STU/WES 75NIC/WAI 60AND/BID 67AND/COI
-Methylph $(1 \times C - (1 \times C_n - 1))$ $(1 \times C_n - 1)$ $(1 \times C_n - 1)$	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	sol ×O-(H)(C _B)) (1×ortho corr) re - Calculated -127.17 130.34 351.10 -313.89 -33.58 13.55 -189.91 225.15 212.58 -452.41 -55.03	+ $(1 \times C_{n}$ - (O) = Residual - 1.43 - 0.01	$(C_B)_2$) + $(C_D)_2$), $\sigma = 3$ Reference 60AND/BID 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{C_{p}^{\circ} - S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ} - C_{p}^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = \frac{\Delta_{t}H^{\circ} - C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \frac{\Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \frac{\Delta_{t}S^{\circ} = C_{t}G^{\circ} $	- 125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29 23.51 - 204.97 153.67 172.40 - 492.59	3.03 0.53 -0.18 0.61	60AND/BIE 69STU/WES 69STU/WES 75NIC/WAI 60AND/BIE 67AND/COI
Methylph $(1 \times C - (1 \times C_n - ($	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	sol × O-(H)(C _B)) (1 × ortho corr) re - Calculated - 127.17 130.34 351.10 - 313.89 - 33.58 13.55 - 189.91 225.15 212.58 - 452.41 - 55.03 22.20	$+ (1 \times C_{n} - (0))$ = Residual -1.43 -0.01 6.51	(C _B) ₂) + (C _D) ₂), σ = 3 Reference 60AND/BID 69STU/WES 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} =$	- 125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29 23.51 - 204.97 153.67 172.40 - 492.59 - 58.11	3.03 0.53 -0.18 0.61	60AND/BII 69STU/WE: 69STU/WE: 75NIC/WAI 60AND/BIE 67AND/CO
Methylph $(1 \times C - (1 \times C_n - ($	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	sol × O-(H)(C _B)) (1 × ortho corr) re - Calculated - 127.17 130.34 351.10 - 313.89 - 33.58 13.55 - 189.91 225.15 212.58 - 452.41 - 55.03 22.20	$+(1 \times C_{n}-(0))$ = Residual -1.43 -0.01 6.51	(C _B) ₂) + (C _D) ₂), σ = 3 Reference 60AND/BID 69STU/WES 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} =$	- 125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29 23.51 - 204.97 153.67 172.40 - 492.59 - 58.11	3.03 0.53 -0.18 0.61	60AND/BII 69STU/WE: 69STU/WE: 75NIC/WAI 60AND/BIE 67AND/CO
Methylph $(1 \times C - (1 \times C_n - (1$	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	sol ×O-(H)(C _B)) (1×ortho corr) re - Calculated -127.17 130.34 351.10 -313.89 -33.58 13.55 -189.91 225.15 212.58 -452.41 -55.03 22.20 -199.97 153.67	+ (1 × C _D -(O) = Residual - 1.43 - 0.01 6.51	(C _B) ₂) + (C _D) ₂), σ = 3 Reference 60AND/BID 69STU/WES 69STU/WES 60AND/BID 67AND/COU	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} =$	- 125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29 23.51 - 204.97 153.67 172.40 - 492.59 - 58.11	3.03 0.53 -0.18 0.61	60AND/BII 69STU/WE: 69STU/WE: 75NIC/WAI 60AND/BIE 67AND/CO
Methylph $(1 \times C_{-1})$ ($1 \times C_{-1}$) ($1 \times C_{-1$	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	sol × O-(H)(C _B)) (1 × ortho corr) re - Calculated - 127.17 130.34 351.10 - 313.89 - 33.58 13.55 - 189.91 225.15 212.58 - 452.41 - 55.03 22.20	$+(1 \times C_{n}-(0))$ = Residual -1.43 -0.01 6.51	(C _B) ₂) + (C _D) ₂), σ = 3 Reference 60AND/BID 69STU/WES 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} =$	- 125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29 23.51 - 204.97 153.67 172.40 - 492.59 - 58.11	3.03 0.53 -0.18 0.61	60AND/BII 69STU/WE: 69STU/WE: 75NIC/WAI 60AND/BIE 67AND/CO
Methylph $(1 \times C - (1))$ as phase $v_t H^o = C_p^o = S_p^o = A_p $	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	sol ×O-(H)(C _B)) (1×ortho corr) re - Calculated -127.17 130.34 351.10 -313.89 -33.58 13.55 -189.91 225.15 212.58 -452.41 -55.03 22.20 -199.97 153.67	+ (1 × C _D -(O) = Residual - 1.43 - 0.01 6.51	(C _B) ₂) + (C _D) ₂), σ = 3 Reference 60AND/BID 69STU/WES 69STU/WES 60AND/BID 67AND/COU	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} =$	- 125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29 23.51 - 204.97 153.67 172.40 - 492.59 - 58.11	3.03 0.53 -0.18 0.61	60AND/BII 69STU/WE 69STU/WE 75NIC/WAI 60AND/BII 67AND/CO
Methylph $(1 \times C_{-1}(1 \times C_{n-1}(1 \times C_{$	H) ₃ (C)) + (1 (C)(C _D) ₂) + Literatu - 128.60 130.33 357.61	sol ×O-(H)(C _B)) (1 × ortho corr) re - Calculated -127.17 130.34 351.10 -313.89 -33.58 13.55 -189.91 225.15 212.58 -452.41 -55.03 22.20 -199.97 153.67 172.40	+ (1 × C _D -(O) = Residual - 1.43 - 0.01 6.51	(C _B) ₂) + (C _D) ₂), σ = 3 Reference 60AND/BID 69STU/WES 69STU/WES 60AND/BID 67AND/COU	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}} =$	- 125.40 124.47 347.65	- 128.43 123.94 347.83 - 317.15 - 33.87 13.66 - 193.17 221.65 212.58 - 452.41 - 58.29 23.51 - 204.97 153.67 172.40 - 492.59 - 58.11	3.03 0.53 -0.18 0.61	60AND/BII 69STU/WE 69STU/WE 75NIC/WA 60AND/BII 67AND/CO

TABLE 15. Alcohols (69) - Continued

2-Ethylphenol $(1 \times C - (H)_3(C)) + (4 \times C_B - (H)(C_B)_2)$ $(1 \times ortho \text{ corr})$			
Literat	ure – Calculated =	Residual	Reference
Gas phase $\Delta_t H^\circ = -145.18$ $C_p^\circ =$	- 148.51 155.95	3.33	63BID/HAN
Liquid phase $ \Delta_t H^\circ = -208.78 $ $ C_p^\circ = S^\circ = \\ \Delta_t S^\circ = \\ \Delta_t G^\circ = \\ \ln K_t = $	-214.72 248.05 259.98 -541.32 -53.33 21.51	5.94	63BID/HAN
3-Ethylphenol (1×C-(H) ₃ (C)) + (4×C _B -(H)(C _B) ₂) (1×meta corr))+(1×C _B (0	

	Literatu	Reference		
Gas phase	e			
$\Delta_{f}H^{\circ} =$	- 146.11	- 150.40	4.29	63BID/HAN
$C_p^{\circ} =$		150.26		
7 to				
$C_p^{\circ} =$	ase -214.30	- 217.98 244.55 259.98	3.68	63BID/HAN
$\Delta_{\mathbf{f}}H^{\circ} = C_{p}^{\circ} = S^{\circ} =$		244.55 259.98	3.68	63BID/HAN
$\Delta_{\mathbf{f}}H^{\circ} = C_{\mathbf{p}}^{\circ} =$		244.55	3.68	63BID/HAN

4-Ethylphenol	C ₈ H ₁₀ O
$(1 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)(C_B)) + (1 \times C_B - (C)(C_B)_2) +$	
$(4 \times C_B - (H)(C_B)_2) + (1 \times O - (H)(C_B)) + (1 \times C_B - (O)(C_B)_2)$	

Literatur	Literature – Calculated = Residual						
Gas phase							
$\Delta_{\rm f}H^{\circ} = -144.10$	- 149.77	5.67	63BID/HAN				
$C_p^{\circ} =$	149.55						
Liquid phase							
$\Delta_0 H^\circ =$	-217.98						
$C_p^{\circ} =$	244.55						
S° =	259.98						
$\Delta_{f}S^{\circ} =$	-541.32						
$\Delta_{\rm f}G^{\circ} =$	-56.59						
$lnK_f =$	22.83						

4-Ethylphenol (Continued)	C ₈ H ₁₀ O
$(1 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)(C_B)) + (1 \times C_B - (C)(C_B))$	2)+
$(4 \times C_B - (H)(C_B)_2) + (1 \times O - (H)(C_B)) + (1 \times C_B - (O)(C_B)_2)$)

;			
- 224.39	-227.07	2.68	63BID/HAN
206.90	203.05	3.85	75NIC/WAD
	199.30		
	-602.00		
	- 47.58		
	19.20		
	- 224.39	- 224.39 - 227.07 206.90 203.05 199.30 - 602.00 - 47.58	-224.39 -227.07 2.68 206.90 203.05 3.85 199.30 -602.00 -47.58

 $\begin{array}{ll} \textbf{2.3-Dimethylphenol} & \textbf{C_{9}H_{10}O} \\ (2 \times \textbf{C}-(\textbf{H})_{3}(\textbf{C})) + (2 \times \textbf{C}_{B}-(\textbf{C})(\textbf{C}_{B})_{2}) + (3 \times \textbf{C}_{B}-(\textbf{H})(\textbf{C}_{B})_{2}) + \\ (1 \times \textbf{O}-(\textbf{H})(\textbf{C}_{B})) + (1 \times \textbf{C}_{B}-(\textbf{O})(\textbf{C}_{B})_{2}) + (2 \times \textit{ortho} \ \textit{corr}) + \\ (1 \times \textit{meta} \ \textit{corr}) \end{array}$

Literatu	re – Calculated	= Residual	Reference
Gas phase			
$\Delta_t H^\circ = -157.19$	- 158.97	1.78	60AND/BID
$C_p^{\circ} =$	159.32		
Liquid phase			
$\Delta_{\mathbf{f}}H^{\circ} =$	-223.26		
<i>C</i> ^o −	252.55		
S° =	247.51		
$\Delta_{i}S^{\circ} =$	-553.79		
$\Delta_t G^{\circ} =$	-58.15		
$lnK_f =$	23.46		
Solid phase			
$\Delta_{\rm r} H^{\circ}241.21$	-232.34	-8.87	60AND/BID
$C_p^{\circ} =$	177.73		
S° =	200.84		
$\Delta_{f}S^{\circ} =$	600.46		
$\Delta_{\mathfrak{l}}G^{\circ} =$	-53.31		
$lnK_f =$	21.51		

 $\begin{array}{ll} \textbf{2,4-Dimethylphenol} & \textbf{C_8H_{10}O} \\ (2 \times C - (H)_3(C)) + (2 \times C_B - (C)(C_B)_2) + (3 \times C_B - (H)(C_B)_2) + \\ (1 \times O - (H)(C_B)) + (1 \times C_B - (O)(C_B)_2) + (1 \times \textit{ortho} \ \textit{corr}) + \\ (1 \times \textit{meta} \ \textit{corr}) \end{array}$

Literatus	Literature – Calculated = Residual					
Gas phase $\Delta_t H^\circ = -162.88$ $C_\rho^\circ =$	- 160.23 152.92	-2.65	60AND/BID			
Liquid phase $\Delta_t H^\circ = -228.78$	-226.52	-2.26	60AND/BID			
$C_p^{\circ} = S^{\circ} =$	249.05 247.51	<i>5.40</i>	007111271212			
$\Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = 0$	-553.79 -61.41 24.77					

2,5-Dimethyl (2×C-(H) (1×C _B -(C) (1×meta)	$(C_B)_2 + (2 \times C_B)_2 + (2 \times C_B)_2$	$\langle C_{B}-(C)(C_{B})_{2}\rangle$ $(3\times C_{B}-(H)(C_{B})_{2})$	$(1 \times O - (H))$ $(1 \times O - (H))$ $(1 \times O - (H))$	$C_aH_{10}O$ $ho (C_B)$) + ho corr) +		$\frac{1}{3}(C) + (2)$ $\frac{1}{3}(C_B) + (1)$	$\times C_{B}$ -(C)(C _B) ₂ $\times C_{B}$ -(O)(C _B)		
	Literature	e – Calculated	= Residual	Reference		Literatui	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 161.59	- 160.23 152.92	-1.36	60AND/BID	Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 156.57	-160.23 152.92	3.66	60AND/BID
Liquid phase $ \Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	ee	- 226.52 249.05 247.51 - 553.79 - 61.41 24.77			Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = S^\circ =$	se	- 226.52 249.05 247.51 - 553.79 - 61.41 24.77		
Solid phase $ \Delta_t H^\circ = C_p^\circ - S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = $	-246.60	-237.34 177.73 200.84 -600.46	- 9.26	60AND/BID	Solid phase $ \Delta_t H^\circ = C_p^\circ - S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S$	- 242.30	-237.34 177.73 200.84 -600.46 -58.31	-4.96	60AND/BID
$\ln K_f =$		-58.31 23.52			$lnK_f =$		23.52		
$\ln K_f =$ 2,6-Dimethy $(2 \times C - (H)^{-1})$	$H_{3}(C) + (2)$ $H_{3}(C_{B}) + (1)$				$lnK_f =$ 3,5-Dimethy $(2 \times C - (H))$	$I_{3}(C) + (2$ $I(C_{B}) + (1$	$\times C_{B}$ -(C)(C _B) ₂ $\times C_{B}$ -(O)(C _B)	$(3 \times meta)$	(C _B) ₂)+ corr)
$\ln K_f =$ 2,6-Dimethy $(2 \times C - (H + (1 \times O - (H + (1 \times O + (H + (1 \times O + (H + $	$H_{3}(C) + (2x)$ $H_{3}(C) + $	23.52 × C _B -(C)(C _B) ₂	$+(2 \times ortho$	$((C_B)_2) +$	$lnK_f =$ 3,5-Dimethy $(2 \times C - (H))$	$I_{3}(C) + (2$ $I(C_{B}) + (1$	× C _B -(C)(C _B) ₂	$(3 \times meta)$	$((C_B)_2) +$
2,6-Dimethy (2 × C-(H (1 × O-(H (1 × meta	$H_{3}(C) + (2x)$ $H_{3}(C) + $	23.52 × C _B -(C)(C _B) ₂ × C _B -(O)(C _B) ₂	$+(2 \times ortho$	()(C _B) ₂)+ corr)+	$lnK_f = {3,5\text{-Dimethy}}$ $(2 \times C - (H)$ $(1 \times O - (H))$ Gas phase	$I_{3}(C) + (2$ $I(C_{B}) + (1$	$\times C_{B}$ -(C)(C _B) ₂ $\times C_{B}$ -(O)(C _B)	$(3 \times meta)$	corr)
$InK_f =$ 2,6-Dimethy (2×C-(H (1×O-(H (1×meta) Gas phase $\Delta_t H^\circ =$	H ₃ (C)) + (2: H)(C _B)) + (1 corr) Literature - 161.80	23.52 × C _B -(C)(C _B) ₂ × C _B -(O)(C _B); e - Calculated - 158.97	n) + (2× <i>ortho</i> = Residual	()(C _B) ₂) + corr) + Reference	$3,5-Dimethy (2 \times C-(H) (1 \times O-(H)))$ Gas phase $\Delta_{\ell}H^{\circ} =$	I) ₃ (C)) + (2 I)(C _B)) + (1 Literatur – 161.59	\times C _B -(C)(C _B) ₂ \times C _B -(O)(C _B) e – Calculated – 162.75	2)+(3×meta)(C _B) ₂)+ corr) Reference

 $\Delta_f G^\circ =$

 $lnK_f =$

 $\Delta_{\rm f} S^{\circ} = \Delta_{\rm f} G^{\circ} =$

 $lnK_f =$

Solid phase $\Delta_t H^\circ = -368.00$ $C_\rho^\circ = 139.33$ $S^\circ =$

-258.74

104.38

-368.38

138.44

151.42

-377.25

-255.90

103.23

0.38

0.89

68DES/WIL

50UEB/ORT

TABLE 15. Alcohols (69) - Continued

TABLE 15. Alcohols (69) - Continued

1,2-Benzenediol; Cated $(2 \times O-(H)(C_B)) + ($		- (4 × C _r (H)	$(C_R)_2$ +	1,4-Benzene (2×O-(]		oquinone 2×C _B -(O)C _B) ₂	+ (4 × C _b -(H)	$\mathbf{C_6H_6O_7}$
(1×OH-OH ortho		(*** 05 (**)	(-8/2)	(= 11 0 (=		re – Calculated		
Literatu	re – Calculated =	Residual	Reference		Literatu		= Residual	Reference
				Gas phase				
Gas phase $\Delta_t H^\circ = -267.50$ $C_p^\circ =$	-268.66 128.88	1.16	84RIB/RIB	$\Delta_t H^\circ = C_p^\circ =$	-265.30	- 274.86 122.48	9.56	56MAG
				Liquid pha	se			
Liquid phase				$\Delta_{\rm f}H^{\circ} =$		-362.08		
$\Delta_{\mathbf{f}}H^{\circ} =$	-358.82			$C_p^{\circ} =$		259.42		
$C_p^{\circ} =$	262.92			S° =		182.08		
S° =	182.08			$\Delta_f S^\circ =$		-449.12		
$\Delta_f S^\circ =$	-449.12			$\Delta_{\mathbf{f}}G^{\circ} =$		-228.18		
$\Delta_{\rm f}G^{\circ} =$	-224.92			$lnK_f =$		92.04		
$lnK_f =$	90.73							
				Solid phase				
Solid phase					-364.50	-370.38	5.88	56PIL/SUT
$\Delta_t H^\circ = -354.10$	-354.38	0.28	84RIB/RIB	$C_p^{\circ} =$	136.40	138.44	-2.04	50UEB/ORT
$C_p^{\circ} = 140.58$	138.44	2.14	50UEB/ORT	S° =		151.42		
S° =	151.42			$\Delta_f S^\circ =$		- 479.78		
$\Delta_{r}S^{\circ} =$	-479.78			$\Delta_t G^\circ =$		-227.33		
$\Delta_i G^{\circ} = $ $ln K_i =$	-211.33 85.25			$lnK_f =$		91.71	· · · · · · · · · · · · · · · · · · ·	
1,3-Benzenediol; Reso	rcinol		C6H6O2	1-Naphthol (7×C _p -(H)(C _n) ₂)+	(1×O−(H)(C _B)))+(1×C₀-((C ₁₉ H ₈ (
$(2 \times O - (H)(C_B)) + (1 \times OH - OH meta)$	$(2 \times C_B - (O)C_B)_2 +$	$+(4\times C_B-(H)$		$(2 \times C_{BF})$	$(C_{BF})(C_B)_2$	$+(1 \times naphtha$	lene 1 sub)	<i>)</i> Св/2 (
	ure – Calculated =	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
				Gas phase				
Gas phase				$\Delta_{\rm f}H^{\circ} =$	-30.80	-28.18	- 2.62	88RIB/RIB
$\Delta_t H^\circ = -274.70$	-274.86	0.16	68DES/WIL	$C_p^* =$		143.68	2.00	
$C_p^{\circ} =$	123.19			<i></i>	·			
Liquid phase	***			Liquid phas	se	100 50		
Liquid phase	262.00			$\Delta_l H^\circ =$		-108.58		
$\Delta_t H^\circ =$	-362.08			$C_p^{\circ} =$		262.15		
$C_p^{\circ} = S^{\circ} =$	259.42			S° =		224.31		
$\Delta_f S^\circ =$	182.08 346.59			$\Delta_f S^\circ = \Delta_f G^\circ =$		~457.90 27.94		
<u>π</u> ω =	- 540.59			$\Delta_{f}U =$		27.94		

 $lnK_{f} =$

 $\Delta_{f}S^{\circ} =$

 $\Delta_t G^\circ =$

 $lnK_f =$

-11.27

-124.34

174.47

177.46

26.15

-10.55

-504.75

88RIB/RIB

2.34

2-Naphthol $(7 \times C_B - (F_B))$ $(2 \times C_{BF} - (F_B))$	$I(C_B)_2 + (C_{BF})(C_B)_2$	1×O-(H)(C _B) +(1×naphtha)+(1×C _B -(0 lene 1 sub)	$C_{10}H_8O$ $O)(C_B)_2) +$	$(8 \times C_B - ($	$(C_{B})_{3}(C) + (2)_{1}(C_{B})_{2} + (2)_{1}(C_{B})_{2}$	$\times C_B - (C)(C_B)_2$	$(2 \times C_B - (O))$ (quaternary))	
	Literatur	e – Calculated :	= Residual	Reference		Litera	ture-Calculate	d = Residual	Reference
Gas phase $\Delta_s H^\circ = C_p^\circ =$	-29.90	- 28.18 143.68	-1.72	88RIB/RIB	Solid phase $\Delta_t H^\circ =$	-368.60	-365.83	- 2.77	48HUB/KNO
Liquid phase	e								
$\Delta_{f}H^{\circ} =$		- 108.58			1,2-Naphtha				C ₁₉ H ₈ O
$C_p^{\circ} =$		262.15			$(6 \times C_B - ($	$H)(C_B)_2) + 0$	$(2 \times O - (H)(C_B)$	$(C_B-(C_B))$	$((C_{B})_{2}) +$
s° =		224.31					+(1×naphtha		
$\Delta_{\mathbf{r}}S^{\circ} =$		-457.90				OH(ortho c		,	
$\Delta_f G^\circ =$		27.94			•	`	,,		
$lnK_f =$		- 11.27				Literatur	e – Calculated	= Residual	Reference
Solid phase					Gas phase				
Solid phase	124.20	_ 124 24	0.14	88RIB/RIB	•	- 200.50	-200.04	_ 0.42	00D1D/D1D
•	- 124.20	- 124.34 174.47	0.14	OONID/KID	-	200.30		-0.43	88RIB/RIB
$C_p^{\circ} =$		174.47			$C_p^{\circ} =$		166.18		
S° =		177.46							
$\Delta_{\mathbf{f}}S^{\circ} =$		-504.75							
$\Delta_{\rm f}G^{\circ} =$		26.15			Liquid phas	ie			
$lnK_f =$		- 10.55			$\Delta_{\rm f}H^{\circ} =$		-314.10		
					$C_p^{\circ} =$		323.82		
					S° =		228.74		
							EEE 00		
					$\Delta_{\mathbf{f}}S^{\circ} =$		- 555.99		
		,3-Dihydroxyna		$C_{10}H_8O_2$	$\Delta_{\rm f}G^{\circ} =$		- 148.33		
(6×C _B -(I	$H)(C_B)_2) + 0$,3-Dihydroxyna (2 × O–(H)(C _B) 1+ (1 × naphtha	$(2 \times C_{B}-(0))$					····	
(6×C _B -(I	$(C_{BF})(C_{B})_{2}$	$(2 \times O - (H)(C_B)$) + (2 × C _B -(0 lene 2 sub)		$\Delta_{\rm f}G^{\circ} =$		- 148.33		
(6×C _B -(I	$(C_{BF})(C_{B})_{2}$	$(2 \times O - (H)(C_B)$ + $(1 \times naphtha$) + (2 × C _B -(0 lene 2 sub)	O)(C _B) ₂) +	$\Delta_t G^\circ = \ln K_t = \frac{1 \ln K_t}{1 + \frac{1}{2} \ln K_t}$ Solid phase $\Delta_t H^\circ = \frac{1}{2} \ln K_t$	- 309.80	-148.33 59.84 -313.12	3.32	88RIB/RIB
(6×C _B -(I	$(C_{BF})(C_{B})_{2}$	$(2 \times O - (H)(C_B)$ + $(1 \times naphtha$) + (2 × C _B -(0 lene 2 sub)	O)(C _B) ₂) +	$\Delta_t G^{\circ} = \ln K_t = \frac{1 \ln K_t}{1 + \frac{1}{2} \ln K_t}$ Solid phase $\Delta_t H^{\circ} = C_p^{\circ} = \frac{1}{2} \ln K_t$		-148.33 59.84	3.32	88RIB/RIB
(6×C _B -(I	$(C_{BF})(C_{B})_{2}$	$(2 \times O - (H)(C_B)$ + $(1 \times naphtha$) + (2 × C _B -(0 lene 2 sub)	O)(C _B) ₂) +	$\Delta_t G^{\circ} = \frac{1}{\ln K_t} = \frac{1}{\ln K_t}$ Solid phase $\Delta_t H^{\circ} = \frac{C_{\rho}^{\circ}}{S^{\circ}} = \frac{1}{\ln K_t}$		-148.33 59.84 -313.12	3.32	88RIB/RIB
(6 × C _B -(I (2 × C _{BF} -($(C_{BF})(C_{B})_{2}$	$(2 \times O-(H)(C_B)$ + $(1 \times naphtha$ e - Calculated - 207.04) + (2 × C _B -(0 lene 2 sub)	O)(C _B) ₂) +	$\Delta_t G^\circ = \frac{1}{\ln K_t} = \frac{1}{\ln K_t}$ Solid phase $\Delta_t H^\circ = \frac{C_t^\circ = S^\circ = \Delta_t S^\circ = \frac{1}{\ln K_t}$		-148.33 59.84 -313.12 183.30	3.32	88RIB/RIB
(6 × C _B -(I (2 × C _{BF} -($(C_B)_2 + (C_B)_2 + (C_B)_2$ Literatur	(2 × O-(H)(C _B) + (1 × naphtha re – Calculated) + (2 × C _B -(0 lene 2 sub) = Residual	O)(C _B) ₂) + Reference	$\Delta_t G^{\circ} = \frac{1}{\ln K_t} = \frac{1}{\ln K_t}$ Solid phase $\Delta_t H^{\circ} = \frac{C_{\rho}^{\circ}}{S^{\circ}} = \frac{1}{\ln K_t}$		- 148.33 59.84 - 313.12 183.30 184.92	3.32	88RIB/RIB
$(6 \times C_{B}-(1 \times C_{B$	$(C_B)_2 + (C_B)_2 + (C_B)_2$ Literatur	$(2 \times O-(H)(C_B)$ + $(1 \times naphtha$ e - Calculated - 207.04) + (2 × C _B -(0 lene 2 sub) = Residual	O)(C _B) ₂) + Reference	$\Delta_t G^\circ = \frac{1}{\ln K_t} = \frac{1}{\ln K_t}$ Solid phase $\Delta_t H^\circ = \frac{C_t^\circ = S^\circ = \Delta_t S^\circ = \frac{1}{\ln K_t}$		- 148.33 59.84 - 313.12 183.30 184.92 - 599.81	3.32	88RIB/RIB
$(6 \times C_{B}-(1 \times C_{BF}-(1 \times $	H)(C _B) ₂) + (C _{BF})(C _B) ₂) Literatur - 192.80	(2 × O-(H)(C _B) + (1 × naphtha e - Calculated - 207.04 166.18) + (2 × C _B -(0 lene 2 sub) = Residual	O)(C _B) ₂) + Reference	$\Delta_t G^\circ = \frac{1}{\ln K_t} = \frac{1}{\ln K_t}$ Solid phase $\Delta_t H^\circ = \frac{C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \frac{1}{\ln K_t}$		- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29	3.32	88RIB/RIB
$(6 \times C_{BF} - (1))$ $(2 \times C_{BF} - (1))$ Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = C_{p}^{\circ} = C_{p}^{\circ}$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = C_{p}^{\circ}$	H)(C _B) ₂) + (C _{BF})(C _B) ₂) Literatur - 192.80	(2 × O-(H)(C _B) + (1 × naphtha re - Calculated - 207.04 166.18) + (2 × C _B -(0 lene 2 sub) = Residual	O)(C _B) ₂) + Reference	Solid phase $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = InK_{t} = InK_{t}$	- 309.80	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29	3.32	
$(6 \times C_{B}-(1 \times C_{BF}-(1 \times $	H)(C _B) ₂) + (C _{BF})(C _B) ₂) Literatur - 192.80	(2 × O-(H)(C _B) + (1 × naphtha re - Calculated - 207.04 166.18 - 314.10 323.82) + (2 × C _B -(0 lene 2 sub) = Residual	O)(C _B) ₂) + Reference	Solid phase $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = InK_{t} = InK_{t}$ 1,3-Naphtha	- 309.80	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17		C ₁₈ H ₈ O ₂
$(6 \times C_{B}-(1 \times C_{BF}-(1 \times $	H)(C _B) ₂) + (C _{BF})(C _B) ₂) Literatur - 192.80	(2 × O-(H)(C _B) + (1 × naphtha re - Calculated - 207.04 166.18 - 314.10 323.82 228.74) + (2 × C _B -(0 lene 2 sub) = Residual	O)(C _B) ₂) + Reference	Solid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = $ 1,3-Naphtha $(6 \times C_{B} - (1))$	-309.80 alenediol H)(C _B) ₂) + (- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17))+(2×C ₈ -(O	C ₁₈ H ₈ O ₂
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = C_{p}^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = C_{p}^{\circ} = C_$	H)(C _B) ₂) + (C _{BF})(C _B) ₂) Literatur - 192.80	(2 × O-(H)(C _B) + (1 × naphtha re - Calculated - 207.04 166.18 - 314.10 323.82 228.74 - 555.99) + (2 × C _B -(0 lene 2 sub) = Residual	O)(C _B) ₂) + Reference	Solid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{1,3-\text{Naphths}}{(6 \times C_{B}-(1)(2 \times C_{BF}-(1)(2 \times C_{B$	- 309.80 alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂)	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2×O-(H)(C _B + (1×naphtha))+(2×C ₈ -(O	C ₁₈ H ₈ O ₂
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = C_{p}^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = C_{p}^{\circ} = C_{$	H)(C _B) ₂) + (C _{BF})(C _B) ₂) Literatur - 192.80	(2 × O-(H)(C _B) + (1 × naphtha re - Calculated - 207.04 166.18 - 314.10 323.82 228.74 - 555.99 - 148.33) + (2 × C _B -(0 lene 2 sub) = Residual	O)(C _B) ₂) + Reference	Solid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{1,3-\text{Naphths}}{(6 \times C_{B}-(1)(2 \times C_{BF}-(1)(2 \times C_{B$	-309.80 alenediol H)(C _B) ₂) + (- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2×O-(H)(C _B + (1×naphtha))+(2×C ₈ -(O	C ₁₈ H ₈ O ₂
Gas phase $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = C_{\rho}^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{$	H)(C _B) ₂) + (C _{BF})(C _B) ₂) Literatur - 192.80	(2 × O-(H)(C _B) + (1 × naphtha re - Calculated - 207.04 166.18 - 314.10 323.82 228.74 - 555.99) + (2 × C _B -(0 lene 2 sub) = Residual	O)(C _B) ₂) + Reference	Solid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{1,3-\text{Naphths}}{(6 \times C_{B}-(1)(2 \times C_{BF}-(1)(2 \times C_{B$	- 309.80 alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2×O-(H)(C _B + (1×naphtha)) + (2 × C _B −(O llene 2 sub) +	C ₁₈ H ₈ O ₂
Gas phase $\Delta_{l}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{l}H^{\circ} = C_{p}^{\circ} =$ $\Delta_{l}G^{\circ} = \Delta_{l}G^{\circ} =$ $\ln K_{f} =$ Solid phase	H)($(C_B)_2$) + ((C_BF) ($(C_B)_2$) Literatur - 192.80	(2 × O-(H)(C _B) + (1 × naphtha re - Calculated - 207.04 166.18 - 314.10 323.82 228.74 - 555.99 - 148.33	1) + (2 × C _B -(0) lene 2 sub) = Residual	O)(C _B) ₂) + Reference	Solid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{1,3-\text{Naphths}}{(6 \times C_{B}-(1)(2 \times C_{BF}-(1)(2 \times C_{B$	- 309.80 alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2×O-(H)(C _B +(1×naphthapprr)))) + (2 × C _B −(O llene 2 sub) +	С ₁₈ Н ₈ О ₂)(С _В)2) +
Gas phase $\Delta_{l}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{l}H^{\circ} = C_{p}^{\circ} =$ $\Delta_{l}G^{\circ} = \Delta_{l}G^{\circ} =$ $\ln K_{f} =$ Solid phase	H)(C _B) ₂) + (C _{BF})(C _B) ₂) Literatur - 192.80	(2 × O-(H)(C _B) + (1 × naphtha re - Calculated - 207.04 166.18 - 314.10 323.82 228.74 - 555.99 - 148.33) + (2 × C _B -(0 lene 2 sub) = Residual	O)(C _B) ₂) + Reference	Solid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{1,3-\text{Naphths}}{(6 \times C_{B}-(1)(2 \times C_{BF}-(1)(2 \times C_{B$	- 309.80 alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2×O-(H)(C _B +(1×naphthapprr)))) + (2 × C _B −(O llene 2 sub) +	С ₁₈ Н ₈ О ₂)(С _В)2) +
Gas phase $\Delta_{l}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{l}H^{\circ} = C_{p}^{\circ} =$ $\Delta_{l}G^{\circ} = \Delta_{l}G^{\circ} =$ $\ln K_{f} =$ Solid phase	H)($(C_B)_2$) + ((C_BF) ($(C_B)_2$) Literatur - 192.80	(2 × O-(H)(C _b) + (1 × naphtha re - Calculated -207.04 166.18 -314.10 323.82 228.74 -555.99 -148.33 59.84	1) + (2 × C _B -(0) lene 2 sub) = Residual	Reference 88RIB/RIB	Solid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = InK_{t} = InK_{t} = InK_{t}$ 1,3-Naphtha $(6 \times C_{B} - (1 \times OH - ($	- 309.80 alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2×O-(H)(C _B +(1×naphthapprr)))) + (2 × C _B −(O llene 2 sub) +	С ₁₈ Н ₈ О ₂)(С _В)2) +
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t G^\circ = \Delta_t G^\circ =$ $\ln K_t =$ Solid phase $\Delta_t H^\circ =$	H)($(C_B)_2$) + ((C_BF) ($(C_B)_2$) Literatur - 192.80	(2 × O-(H)(C _b) + (1 × naphtha re - Calculated - 207.04 166.18 - 314.10 323.82 228.74 - 555.99 - 148.33 59.84	1) + (2 × C _B -(0) lene 2 sub) = Residual	Reference 88RIB/RIB	Solid phase $\Delta_t H^\circ = C_p^\circ = S_0 $	alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2×O-(H)(C _B) + (1×naphthaperr)) e - Calculated)) + (2 × C _B -(O llene 2 sub) + = Residual	$C_{10}H_8O_2$)(C_B) $_2$) + Reference
$(6 \times C_{B}-(1))$ $(2 \times C_{BF}-(1))$ $C_{A} = C_{A} =$	H)($(C_B)_2$) + ((C_BF) ($(C_B)_2$) Literatur - 192.80	(2 × O-(H)(C _b) + (1 × naphtha re - Calculated - 207.04 166.18 - 314.10 323.82 228.74 - 555.99 - 148.33 59.84 - 329.12 183.30	1) + (2 × C _B -(0) lene 2 sub) = Residual	Reference 88RIB/RIB	Solid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = InK_{t} = InK_{t} = InK_{t}$ 1,3-Naphtha $(6 \times C_{B} - (1 \times OH - ($	alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2×O-(H)(C _B) + (1×naphthaperr)) e - Calculated)) + (2 × C _B -(O llene 2 sub) + = Residual	$C_{10}H_8O_2$)(C_B) $_2$) + Reference
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ $\Delta_{t}G^{\circ} = $ $\Delta_{t}G^{\circ} = $ $\ln K_{t} = $ Solid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ $C_{p}^{\circ} = C_{p}^{\circ} = $	H)($(C_B)_2$) + ((C_BF) ($(C_B)_2$) Literatur - 192.80	(2 × O-(H)(C _b) + (1 × naphtha re - Calculated - 207.04 166.18 - 314.10 323.82 228.74 - 555.99 - 148.33 59.84 - 329.12 183.30 184.92	1) + (2 × C _B -(0) lene 2 sub) = Residual	Reference 88RIB/RIB	Solid phase $\Delta_t H^\circ = C_p^\circ = S_0 $	alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2×O-(H)(C _B) + (1×naphthaperr)) e - Calculated)) + (2 × C _B -(O llene 2 sub) + = Residual	$C_{10}H_8O_2$)(C_B) $_2$) + Reference
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = C_{p}^{\circ} = \Delta_{t}G^{\circ} $	H)($(C_B)_2$) + ((C_BF) ($(C_B)_2$) Literatur - 192.80	- 207.04 166.18 - 314.10 323.82 228.74 - 555.99 - 148.33 59.84 - 329.12 183.30 184.92 - 599.81 - 150.29	1) + (2 × C _B -(0) lene 2 sub) = Residual	Reference 88RIB/RIB	Solid phase $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = InK_{t} = InK_{t} = InK_{t}$ 1,3-Naphtha $(6 \times C_{B} - (1 \times OH - 1))$ Gas phase $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = InK_{t} = C_{\rho}^{\circ} = InK_{t}$	- 309.80 alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2×O-(H)(C _B) + (1×naphthaperr)) e - Calculated)) + (2 × C _B -(O llene 2 sub) + = Residual	$C_{10}H_8O_2$)(C_B) $_2$) + Reference
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = C_{p}^{\circ} = \Delta_{t}G^{\circ} =$	H)($(C_B)_2$) + ((C_BF) ($(C_B)_2$) Literatur - 192.80	- 207.04 166.18 - 314.10 323.82 228.74 - 555.99 - 148.33 59.84 - 329.12 183.30 184.92 - 599.81	1) + (2 × C _B -(0) lene 2 sub) = Residual	Reference 88RIB/RIB	Solid phase $\Delta_{t}H^{\circ} = C^{\circ}_{\rho} = S^{\circ} = \Delta_{t}S^{\circ} = InK_{t} = InK_{t}$ 1,3-Naphtha $(6 \times C_{B^{-}}(1 \times OH^{-1}))$ Gas phase $\Delta_{t}H^{\circ} = C^{\circ}_{\rho} = InK_{t} = InK_{t}$ Using the solution of the second se	- 309.80 alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2 × O-(H)(C _B , + (1 × naphtha orr)) e - Calculated - 207.04 166.18)) + (2 × C _B -(O llene 2 sub) + = Residual	$C_{10}H_8O_2$)(C_B) $_2$) + Reference
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = C_{p}^{\circ} = \Delta_{t}G^{\circ} $	H)($(C_B)_2$) + ((C_BF) ($(C_B)_2$) Literatur - 192.80	- 207.04 166.18 - 314.10 323.82 228.74 - 555.99 - 148.33 59.84 - 329.12 183.30 184.92 - 599.81 - 150.29	1) + (2 × C _B -(0) lene 2 sub) = Residual	Reference 88RIB/RIB	Solid phase $\Delta_{t}H^{\circ} = C^{\circ}_{p} = S^{\circ} = \Delta_{t}S^{\circ} = InK_{t} = InK_{t} = InK_{t}$ 1,3-Naphtha $(6 \times C_{B} - (1 \times OH - 1))$ Gas phase $\Delta_{t}H^{\circ} = C^{\circ}_{p} = InUnit In $	- 309.80 alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2×O-(H)(C _B + (1×naphtha orr)) e - Calculated - 207.04 166.18)) + (2 × C _B -(O llene 2 sub) + = Residual	$C_{10}H_8O_2$)(C_B) $_2$) + Reference
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = C_{p}^{\circ} = \Delta_{t}G^{\circ} $	H)($(C_B)_2$) + ((C_BF) ($(C_B)_2$) Literatur - 192.80	- 207.04 166.18 - 314.10 323.82 228.74 - 555.99 - 148.33 59.84 - 329.12 183.30 184.92 - 599.81 - 150.29	1) + (2 × C _B -(0) lene 2 sub) = Residual	Reference 88RIB/RIB	Solid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = InK_{t} = InK$	- 309.80 alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2 × O-(H)(C _B , + (1 × naphtha orr)) e - Calculated - 207.04 166.18 - 314.10 323.82)) + (2 × C _B -(O llene 2 sub) + = Residual	$C_{10}H_8O_2$)(C_B) $_2$) + Reference
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = C_{p}^{\circ} = \Delta_{t}G^{\circ} $	H)($(C_B)_2$) + ((C_BF) ($(C_B)_2$) Literatur - 192.80	- 207.04 166.18 - 314.10 323.82 228.74 - 555.99 - 148.33 59.84 - 329.12 183.30 184.92 - 599.81 - 150.29	1) + (2 × C _B -(0) lene 2 sub) = Residual	Reference 88RIB/RIB	Solid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S_{0}^{\circ} = S_{$	- 309.80 alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2 × O-(H)(C _B , + (1 × naphtha orr)) e - Calculated - 207.04 166.18 - 314.10 323.82 228.74)) + (2 × C _B -(O llene 2 sub) + = Residual	$C_{10}H_8O_2$)(C_B) $_2$) + Reference
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = C_{p}^{\circ} = \Delta_{t}G^{\circ} $	H)($(C_B)_2$) + ((C_BF) ($(C_B)_2$) Literatur - 192.80	- 207.04 166.18 - 314.10 323.82 228.74 - 555.99 - 148.33 59.84 - 329.12 183.30 184.92 - 599.81 - 150.29	1) + (2 × C _B -(0) lene 2 sub) = Residual	Reference 88RIB/RIB	Solid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S_{0}^{\circ}$ $\Delta_{t}G^{\circ} = S_{0}^{\circ} = S_{0}^{\circ} = S_{0}^{\circ}$ $\Delta_{t}G^{\circ} = S_{0}^{\circ} = S_{0}^{\circ}$ $S^{\circ} = S_{0}^{\circ} = S_{0}^{\circ} = S_{0}^{\circ}$ $S^{\circ} = S_{0}^{\circ} = S_{0}^{\circ}$ $S^{\circ} = S_{0}^{\circ} = S_{0}^{\circ} = S_{0}^{\circ} = S_{0}^{\circ} = S_{0}^{\circ}$	- 309.80 alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2×O-(H)(C _B + (1×naphthaper)) e - Calculated - 207.04 166.18 - 314.10 323.82 228.74 - 555.99)) + (2 × C _B -(O llene 2 sub) + = Residual	$C_{10}H_8O_2$)(C_B) $_2$) + Reference
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = C_{p}^{\circ} = \Delta_{t}G^{\circ} $	H)($(C_B)_2$) + ((C_BF) ($(C_B)_2$) Literatur - 192.80	- 207.04 166.18 - 314.10 323.82 228.74 - 555.99 - 148.33 59.84 - 329.12 183.30 184.92 - 599.81 - 150.29	1) + (2 × C _B -(0) lene 2 sub) = Residual	Reference 88RIB/RIB	Solid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S_{0}^{\circ} = S_{$	- 309.80 alenediol H)(C _B) ₂) + ((C _{BF})(C _B) ₂) OH(meta co	- 148.33 59.84 - 313.12 183.30 184.92 - 599.81 - 134.29 54.17 (2 × O-(H)(C _B , + (1 × naphtha orr)) e - Calculated - 207.04 166.18 - 314.10 323.82 228.74)) + (2 × C _B -(O llene 2 sub) + = Residual	$C_{10}H_8O_2$)(C_B) $_2$) + Reference

TABLE 15. Alcohols (69) - Continued

TABLE 16. Ethers (53)

1,3-Naphthalenediol (Continued) $(6 \times C_B - (H)(C_B)_2) + (2 \times O - (H)(C_B)) + (2 \times C_B - (O(B)_2) + (2 \times O(B)_2) + (2 \times O(B$	$C_{10}H_8O_2$ $(C_B)_2) +$	Methoxyme (2×C-(I		ethyl ether ×O-(C)2), σ :	= 18	C₂H.	
$(2 \times C_{BF} - (C_{BF})(C_B)_2) + (1 \times naphthalene \ 2 \ sub) + (1 \times OH - OH(meta \ corr)$					= Residual	ual Reference	
Literature – Calculated = Residual	Reference	Gas phase				***	
Folid phase $ \Delta_t H^\circ = -327.20 -327.12 -0.08 $ $ C_t^\circ = 183.30 $ $ S^\circ = 184.92 $ $ \Delta_t S^\circ = -599.81 $ $ \Delta_t G^\circ = -148.29 $ $ \ln K_t = 59.82 $	88RIB/RIB	$\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{f} =$	-184.10 65.81 267.06	- 185.94 70.00 259.94 - 245.78 - 112.66 45.45	1.84 -4.19 7.12	64PIL/PEL 69STU/WES 69STU/WES	
		Ethoxyetha			×C (II) (O)(C4H16	
,4-Naphthalenediol $(6 \times C_B - (H)(C_B)_2) + (2 \times O - (H)(C_B)) + (2 \times C_B - (O \times C_B)_2) + (1 \times C_B + (O \times C_B)_2) + (1 $	$C_{16}H_8O_2$ $O((C_B)_2) +$,,	×O-(C) ₂)+(2 re – Calculated		Reference	
Literature - Calculated = Residual	Reference	Gas phase $\Delta_t H^\circ =$	- 252.10	- 251.74	-0.36	63PIL/SKI	
Gas phase $C_p = -197.00 -207.04$ 10.04 $C_p^{\circ} = 166.18$	88RIB/RIB	$C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = 0$	112.51 342.67	110.66 346.80 -431.54 -123.08 49.65	1.85 -4.13	69STU/WES 69STU/WES	
iquid phase $\Delta_t H^{\circ} = -314.10$		Liquid phas					
$C_p^o = 323.82$ $S^o = 228.74$ $\Delta_t S^o = -555.99$ $\Delta_t G^o = -148.33$ $\ln K_t = 59.84$			- 279.40 172.51 253.50	-277.65 164.51 258.56 -519.78 -122.68 49.49	- 1.75 8.00 - 5.06	71COU/LEE 71COU/LEE 71COU/LEE	
olid phase $\Delta_t H^\circ = -317.40 -329.12$ 11.72 $C_p^\circ = 183.30$ $S^\circ = 184.92$ $\Delta_t S^\circ = -599.81$	88RIB/RIB	(2×C-(I		-propyl ether \times O-(C) ₂)+(2 σ = 18	× C-(H) ₂ (C) ₂)	C ₆ H ₁ .	
$\Delta_t G^{\circ} = -150.29$ $\ln K_t = 60.62$			Literatu	re – Calculated	= Residual	Reference	
		Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = 0$	- 293.10 158.28 422.50	- 293.00 156.44 425.12 - 625.84 - 106.41 42.92	-0.10 1.84 -2.62	80MAJ/WAG 69STU/WES 69STU/WES	
		Liquid phas $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0 $	se 328.82 221.58 323.88	-329.11 225.35 323.32 -727.64 -112.16 45.25	0.29 - 3.77 0.56	65COL/PEL 75AND/COU 75AND/COU	

		\times C-(H) ₂ (C) ₂) +	(2×C-(H) ₂	$C_8H_{18}O$ $(O)(C)) +$	(2×C-(I		yl butyl ether 2×C-(H) ₂ (C) ₂) ·	+ (1 × C-(H) ₂	$C_5H_{12}C_{1}(O)(C)) +$
	Literatu	re – Calculated =	Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-332.90 204.01 500.41	-334.26 202.22 503.44 -820.14 -89.73 36.20	1.36 1.79 -3.03	80MAJ/WAG 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-258.10	-260.10 136.11 387.45 -527.20 -102.92 41.52	2.00	75FEN/HAR
Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	se -377.90	-380.57 286.19 388.08 -935.50 -101.65 41.01	2.67	65COL/PEL	Liquid pha $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se 290.60 192.72 295.30	- 293.31 191.71 290.73 - 623.92 - 107.29 43.28	2.71 1.01 4.57	75FEN/HAR 75AND/MAR 75AND/MAR
		el ethyl ether ×C-(H)2(O)(C)))+(1×O-(0	C_3H_8O C_2), $\sigma = 9$	(2×C-(I		yl decyl ether $1 \times C - (H)_2(O)(C)$ = 9))+(1×O-((C ₁₁ H ₂₄ O C) ₂) +
	Literatu	re – Calculated =	Residual	Reference	an Kan	Literatu	re – Calculated =	= Residual	Reference
Gas phase $\Delta_i H^o =$ $C_p^o =$ $S^o =$ $\Delta_t S^o =$ $\Delta_t G^o =$ $\ln K_t =$	216.40 89.75 310.62	-218.84 90.33 309.13 -332.89 -119.59 48.24	2.44 -0.58 1.49	64PIL/PEL 69STU/WES 69STU/WES	Gas phase $ \Delta_t H^o = C_p^o = S^o = \Delta_t S^o = \Delta_t G^o = \ln K_t = $	- 381.12	- 383.88 273.45 622.41 - 1110.10 - 52.90 21.34	2.76	75FEN/HAR
(2×C-(I	$(C)_{3}(C) + (1)_{3}(C)_{2}, \sigma = 9$	hyl propyl ether \times C-(H) ₂ (C) ₂) + re - Calculated =	. , ,-	C ₄ H ₁₀ O (O)(C)) + Reference	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se - 443.42 370.80 490.50	-447.69 374.23 485.01 -1247.50 -75.75 30.56	4.27 -3.43 5.49	75FEN/HAR 75AND/MAR 75AND/MAR
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-237.70 112.51 349.45	- 239.47 113.22 348.29 - 430.05 - 111.25 44.88	1.77 -0.71 1.16	64PIL/PEL 69STU/WES 69STU/WES	(3×C-(H (1×C-(H	$H)_3(C)) + (1$ $H)(O)(C)_2$ (H corr (terti	ethyl isopropyl ε × O-(C) ₂) + ethers,esters)) + iary)), σ = 27		C₄H ₁₆ O Reference
Liquid phas $ \Delta_t H^\circ = C_t^\circ - S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t - K_t^\circ $	se - 265.89 161.90 253.70	-267.58 161.29 258.35 -519.99 -112.55 45.40	1.69 0.61 -4.65	80MAJ/WAG 75AND/MAR 75AND/MAR	Gas phase $ \Delta_t H^\circ \sim C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ \sim \ln K_t = S^\circ = S$	- 252.00 111.09 338.32	-252.18 113.51 331.09 -447.25 -118.83 47.94	0.18 - 2.42 7.23	64PIL/PEL 69STU/WES 69STU/WES

TABLE 16. Ethers (53) - Continued

(3×C-(1 (1×C-(1	$H)_3(C)) + (1)$ $H)(O)(C)_2$	thyl isopropyl $(\times O - (C)_2) + (C)_2$ ethers, esters) $(\times O - (C)_2) + (C)_2$		ued) C ₄ H ₁₀ O	(4×C-(I	H) ₃ (C)) + (2 C) ₂) + (4 × -	Diisopropyl eth 2×C-(H)(O)(C -CH ₃ corr (tert	$(c)_2$ (ethers, esteriory)), $\sigma = 16$	2
	Literatur	e – Calculated :	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	- 278.70 161.92 253.72	-279.02 159.27 251.37 -526.97 -121.90 49.18	0.32 2.65 2.35	80MAJ/WAG 75AND/MAR 75AND/MAR	Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f = $	-319.40 158.28 390.24	-318.42 157.02 390.71 -660.25 -121.57 49.04	- 0.98 1.26 - 0.47	80MAJ/WAG 69STU/WES 69STU/WES
butyl etl (4×C-(her (H) ₃ (C)) + (1 H ₃ corr (quat	ropane; Methyl \times C-(O)(C) ₃ (6 iernary)), $\sigma =$	thers,esters)) 243	$C_3H_{12}O$ + $(1 \times O - (C)_2)$ + Reference	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se - 351.50 216.10 304.60	-351.99 221.31 309.36 -741.60 -130.88 52.80	0.49 - 5.21 - 4.76	65COL/PEL 74AND/COU 74AND/COU
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 283.50 134.18 352.96	- 274.64 136.06 351.02 - 563.63 - 106.59 43.00	-8.86 -1.88 1.94	80MAJ/WAG 69STU/WES 69STU/WES	(4×C-(F (2×C-(F	$H_{3}(C) + (2H_{3}(C)) + (2H$	-sec-butyl ether $C \times C - (H)_2(C)_2$ (ethers, esters)) iary)), $\sigma = 162$ re - Calculated	+ + (1 × O-(C) ₂) }	C ₈ H ₁₈ O + Reference
Liquid phate $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	ase - 313.60 187.50 265.30	-313.65 190.65 265.30 -649.35 -120.05 48.43	0.05 -3.15 0.00	75FEN/HAR 75AND/MAR 75AND/MAR	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t =$	- 360.70 204.01 462.62	- 355.16 202.80 469.03 - 854.55 - 100.38 40.49	- 5.54 1.21 - 6.41	80MAJ/SVO 69STU/WES 69STU/WES
(2×C-($(C)_2), \sigma = 9$	\times C-(H) ₂ (C) ₂)		C ₅ H ₁₂ O (O)(C)) +	Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	se 401.50	- 399.09 282.15 374.12 - 949.46	- 2.41	65COL/PEL
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 272.21	- 272.37 133.55 391.72 - 522.93 - 116.46 46.98	0.16	75FEN/HAR	$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = \\ -$	· .	- 116.01 46.80		
Liquid ph. $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	ase - 303.59 197.20 295.00	- 303.38 194.93 290.94 - 623.71 - 117.42 47.37	- 0.21 2.27 4.06	75FEN/HAR 75AND/MAR 75AND/MAR					

(1×C-(1	$H)(O)(C)_2$	ethers,esters))	ropyl tert-buty ethers,esters)) + (1×O-(C) ₂)	+			$\times C_{d-}(H)_2) + ($ $\times C_{d-}(O)(H))$	1×C-(H) ₂ (O)((C))+
(3×-CH	l₃ corr (terti l₃ corr (quat	ernary)), σ =	729			Literatu	re – Calculated	= Residual	Reference
	Literatur	e – Calculated	= Residual	Reference	Complete				
				- <u> </u>	Gas phase $\Delta_t H^\circ = -$	140.16	-141.85	1.69	63PIL/SKI
Gas phase			4404	**************************************					
$\Delta_{\rm f}H^{\circ} =$	-357.73	-340.88	- 16.85	70COX/PIL	Timid above				
$C_p^{\circ} =$	181.17	179.57	1.60	69STU/WES	Liquid phase		- 164.33	2 22	70COV/DII
S° =	417.94	416.40	1.54	69STU/WES	•	166.65	- 164.33 174.30	-2.32	70COX/PIL
$\Delta_f S^\circ =$		- 770.87			$C_p^{\circ} =$		174.30		
$\Delta_{\rm f}G^{\circ} =$		111.05							
$lnK_f =$		44.80							
					Butoxyethene	; n-Butyl	vinyl ether		C ₆ H ₁₂ O
Liquid pha	ase				$(1 \times C_d - (H))$	$)_{2})+(1\times$	C_{d} – $(O)(H))+($	$1 \times O - (C)(C_d)$	+
$\Delta_t H^\circ =$	-392.88	-386.62	-6.26	61SMU/BON	$(1 \times C - (H))$	₂ (O)(C))	+ (2 × C-(H) ₂ ($C)_2$) + (1 × C-(F	I)₃(C))
$C_p^{\circ} =$		252.69							
S° =		323.29				Literatu	re – Calculated	= Residual	Reference
Δ _f S° =		- 863.98						· · · · · · · · · · · · · · · · · · ·	
$\Delta_f G^\circ =$		- 129.02							
$lnK_f =$		52.05			Gas phase $\Delta_t H^\circ = -$	184.50	- 183.11	- 1.39	81TRO/NED
			····				100.11		
(2-Methyl)	propoxy-2-(2-methyl)props	ane; Di-						
tert-buty				C ₈ H ₁₈ O	Liquid phase				
				(ethers,esters)) +	-	218.80	-215.79	-3.01	81TRO/NED
(6×-CI	H ₃ corr (qua	ternary)), σ =	13122		$C_p^{\circ} =$	231.79	235.14	- 3.35	47SCH/ZOS
	Literatu	re – Calculated	l = Residual	Reference					
	`								
Gas nhase					Dimethoxyme		' × O-(C)-) + (1	х С - (Н)-(О)-)	
Gas phase Δ _t H° =		-363.34	1.34	75FEN/HAR	•		×O-(C) ₂)+(1	× C-(H) ₂ (O) ₂)	
$\Delta_t H^{\circ} =$	-362.00	-363.34 202.12	1.34 1.89	75FEN/HAR 69STU/WES	•	₃ (C))+(2	. , , .		
$\Delta_t H^{\circ} = C_p^{\circ} =$	-362.00 204.01	202.12	1.89	69STU/WES	•	₃ (C))+(2	:×O-(C) ₂)+(1		
$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} =$	-362.00	202.12 430.57			•	₃ (C))+(2	. , , .		
$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = 0$	-362.00 204.01	202.12	1.89	69STU/WES	(2×C-(H)	₃ (C))+(2	. , , .		
$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} =$	-362.00 204.01	202.12 430.57 -893.01	1.89	69STU/WES	(2×C-(H))	₃ (C))+(2	. , , .		
$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = S^{\circ} $	-362.00 204.01	202.12 430.57 - 893.01 - 97.09	1.89	69STU/WES	(2×C-(H))	Literatur	re – Calculated	= Residual	Reference
$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = S^{\circ} $	- 362.00 204.01 427.27	202.12 430.57 - 893.01 - 97.09	1.89	69STU/WES	(2×C-(H))	Literatur - 348.20	re – Calculated	= Residual	Reference
$\Delta_t H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1}{2}$	- 362.00 204.01 427.27	202.12 430.57 - 893.01 - 97.09	1.89	69STU/WES	$(2 \times C - (H))$ Gas phase $\Delta_t H^\circ = -$ Liquid phase	Literatur - 348.20	re – Calculated	= Residual	Reference
$\Delta_t H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = -$ Liquid ph	-362.00 204.01 427.27	202.12 430.57 - 893.01 - 97.09 39.17	1.89 -3.30	69STU/WES 69STU/WES	$(2 \times C - (H))$ Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_t^\circ = -$	Literatur - 348.20	re – Calculated – 349.58	= Residual	Reference 69PIL/FLE
$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1}{2}$ Liquid phi $\Delta_t H^{\circ} = \frac{1}{2}$	-362.00 204.01 427.27 ase -399.61	202.12 430.57 -893.01 -97.09 39.17	1.89 -3.30	69STU/WES 69STU/WES 75FEN/HAR	$(2 \times C - (H))$ Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$	Literatur - 348.20	- 349.58 - 379.77	1.38	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL
$\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{2}$ Liquid ph. $\Delta_t H^\circ = C_\rho^\circ = \frac{1}{2}$	-362.00 204.01 427.27 ase -399.61	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07	1.89 -3.30	69STU/WES 69STU/WES 75FEN/HAR	$(2 \times C - (H))$ Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_t^\circ = -$	3(C)) + (2 Literature 348.20 -378.20 161.42	- 349.58 - 379.77 161.42	1.38	Reference 69PIL/FLE 70BIR/SKI
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{2}$ Liquid photograph $\Delta_t H^\circ = C_p^\circ = S^\circ = \frac{1}{2}$	-362.00 204.01 427.27 ase -399.61	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22	1.89 -3.30	69STU/WES 69STU/WES 75FEN/HAR	$(2 \times C - (H))$ Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_t^\circ = -$ $S^\circ = -$	3(C)) + (2 Literature 348.20 -378.20 161.42	- 349.58 - 379.77 161.42 244.01	1.38	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{2}$ Liquid phi $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \frac{1}{2}$	-362.00 204.01 427.27 ase -399.61	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36	1.89 -3.30	69STU/WES 69STU/WES 75FEN/HAR	$(2 \times C - (H))$ Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_t^\circ = -$ $S^\circ = -$ $\Delta_t S^\circ = -$	3(C)) + (2 Literature 348.20 -378.20 161.42	- 349.58 - 379.77 161.42 244.01 - 500.54	1.38	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{2}$ Liquid phi $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \frac{1}{2}$	-362.00 204.01 427.27 ase -399.61	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36 - 127.17	1.89 -3.30	69STU/WES 69STU/WES 75FEN/HAR	$(2 \times C - (H))$ Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_t^\circ = -$ $S^\circ = -$ $\Delta_t S^\circ = -$ $\Delta_t G^\circ = -$	3(C)) + (2 Literature 348.20 -378.20 161.42	- 349.58 - 379.77 161.42 244.01 - 500.54 - 230.53	1.38	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1}{2}$ Liquid phi $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \frac{1}{2}$	-362.00 204.01 427.27 ase -399.61	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36 - 127.17	1.89 -3.30	69STU/WES 69STU/WES 75FEN/HAR	$(2 \times C - (H))$ Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_t^\circ = -$ $S^\circ = -$ $\Delta_t S^\circ = -$ $\Delta_t G^\circ = -$	3(C))+(2 Literature 348.20 -378.20 161.42 244.01	- 349.58 - 379.77 161.42 244.01 - 500.54 - 230.53	1.38	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL 64MCE/KIL
$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = S_0^{\circ} = \Delta_t G^{\circ} = InK_t = InK_t = InK_t = S^{\circ} = S^{\circ} = \Delta_t G^{\circ} = InK_t = InK_$	-362.00 204.01 427.27 ase -399.61 276.10	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36 - 127.17	1.89 -3.30	69STU/WES 69STU/WES 75FEN/HAR	Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_p^\circ = S^\circ = $ $\Delta_t S^\circ = $ $\ln K_t = $ Trimethoxym	348.20 378.20 161.42 244.01	- 349.58 - 379.77 161.42 244.01 - 500.54 - 230.53 93.00	1.38 1.57 0.00 0.00	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL 64MCE/KIL
$\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid ph. $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = $ 1,1'-Oxybi	- 362.00 204.01 427.27 ase - 399.61 276.10	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36 - 127.17 51.30	1.89 -3.30 21.64 -7.97	69STU/WES 69STU/WES 75FEN/HAR 75FEN/HAR	Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_p^\circ = S^\circ = $ $\Delta_t S^\circ = $ $\ln K_t = $ Trimethoxym	348.20 378.20 161.42 244.01	- 349.58 - 379.77 161.42 244.01 - 500.54 - 230.53	1.38 1.57 0.00 0.00	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL
$\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid ph. $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = $ 1,1'-Oxybi	-362.00 204.01 427.27 ase -399.61 276.10	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36 - 127.17 51.30 - 127.17 51.30	1.89 -3.30 21.64 -7.97 Divinyl ether	69STU/WES 69STU/WES 75FEN/HAR 75FEN/HAR C4H60	Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_p^\circ = S^\circ = $ $\Delta_t S^\circ = $ $\ln K_t = $ Trimethoxym	348.20 348.20 378.20 161.42 244.01	- 349.58 - 379.77 161.42 244.01 - 500.54 - 230.53 93.00	1.38 1.57 0.00 0.00 × C-(H)(O) ₃)	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL 64MCE/KIL
$\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid ph. $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = $ 1,1'-Oxybi	-362.00 204.01 427.27 ase -399.61 276.10	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36 - 127.17 51.30	1.89 -3.30 21.64 -7.97 Divinyl ether	69STU/WES 69STU/WES 75FEN/HAR 75FEN/HAR	Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_p^\circ = S^\circ = $ $\Delta_t S^\circ = $ $\ln K_t = $ Trimethoxym	348.20 348.20 378.20 161.42 244.01	- 349.58 - 379.77 161.42 244.01 - 500.54 - 230.53 93.00 × O-(C) ₂) + (1	1.38 1.57 0.00 0.00 × C-(H)(O) ₃)	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL 64MCE/KIL
$\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid ph. $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = $ 1,1'-Oxybi	-362.00 204.01 427.27 ase -399.61 276.10	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36 - 127.17 51.30 - 127.17 51.30	1.89 -3.30 21.64 -7.97 Divinyl ether	69STU/WES 69STU/WES 75FEN/HAR 75FEN/HAR C4H60	Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_p^\circ = S^\circ = $ $\Delta_t S^\circ = $ $\ln K_t = $ Trimethoxym	348.20 348.20 378.20 161.42 244.01	- 349.58 - 379.77 161.42 244.01 - 500.54 - 230.53 93.00 × O-(C) ₂) + (1	1.38 1.57 0.00 0.00 × C-(H)(O) ₃)	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL 64MCE/KIL
$\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid ph. $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = $ 1,1'-Oxybi	- 362.00 204.01 427.27 ase - 399.61 276.10 isethene; Eth -(H) ₂) + (1 × Literatu	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36 - 127.17 51.30 - 127.17 51.30	1.89 -3.30 21.64 -7.97 Divinyl ether	69STU/WES 69STU/WES 75FEN/HAR 75FEN/HAR C4H60	Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_p^\circ = S^\circ = $ $\Delta_t S^\circ = $ $\Delta_t G^\circ = $ $\ln K_t = $ Trimethoxym $(3 \times C - (H))$	348.20 -378.20 161.42 244.01 ethane 3(C)) + (3	- 349.58 - 379.77 161.42 244.01 - 500.54 - 230.53 93.00 × O-(C) ₂) + (1	1.38 1.57 0.00 0.00 × C-(H)(O) ₃)	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL 64MCE/KIL
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1,1'-Oxybi}{2 \times C_0}$	- 362.00 204.01 427.27 ase - 399.61 276.10 isethene; Eth -(H) ₂) + (1 × Literatu	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36 - 127.17 51.30 - 127.17 51.30	1.89 -3.30 21.64 -7.97 Divinyl ether	69STU/WES 69STU/WES 75FEN/HAR 75FEN/HAR C4H60	Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t = $ Trimethoxym $(3 \times C - (H))$ Gas phase	348.20 -378.20 161.42 244.01 ethane 3(C)) + (3	- 349.58 - 379.77 161.42 244.01 - 500.54 - 230.53 93.00 × O-(C) ₂) + (1	1.38 1.57 0.00 0.00 × C-(H)(O) ₃) = Residual	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL 64MCE/KIL C4H10O3
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1,1'-Oxybi}{(2 \times C_d^\circ)}$	- 362.00 204.01 427.27 ase - 399.61 276.10 sethene; Eth-(H) ₂) + (1 × Literatu	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36 - 127.17 51.30 - 127.17 51.30 - 127.17 - 12.25 - 127.17 - 127.17	1.89 -3.30 21.64 -7.97 Divinyl ether < C _d -(O)(H)) i = Residual	69STU/WES 69STU/WES 75FEN/HAR 75FEN/HAR C4H60 Reference	Gas phase $\Delta_{t}H^{\circ} = -$ Liquid phase $\Delta_{t}H^{\circ} = -$ $C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = $ $\Delta_{t}G^{\circ} = $ $\ln K_{t} = $ Trimethoxym $(3 \times C - (H))$ Gas phase $\Delta_{t}H^{\circ} = -$	348.20 348.20 378.20 161.42 244.01 ethane 3(C)) + (3 Literatur 545.00	- 349.58 - 379.77 161.42 244.01 - 500.54 - 230.53 93.00 × O-(C) ₂) + (1	1.38 1.57 0.00 0.00 × C-(H)(O) ₃) = Residual	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL 64MCE/KIL C4H10O3
$\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t = \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_$	-362.00 204.01 427.27 ase -399.61 276.10 isethene; Eth-(H) ₂) + (1 × Literatu	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36 - 127.17 51.30 - 127.17 51.30 - 127.17 - 12.25 - 127.17 - 127.17	1.89 -3.30 21.64 -7.97 Divinyl ether < C _d -(O)(H)) i = Residual	69STU/WES 69STU/WES 75FEN/HAR 75FEN/HAR C4H60 Reference	Gas phase $\Delta_{t}H^{\circ} = -$ Liquid phase $\Delta_{t}H^{\circ} = -$ $C_{p}^{\circ} = $ $S^{\circ} = $ $\Delta_{t}S^{\circ} = $ $\ln K_{t} = $ Trimethoxym $(3 \times C - (H))$ Gas phase $\Delta_{t}H^{\circ} = -$ Liquid phase	348.20 -378.20 161.42 244.01 ethane 3(C)) + (3 Literatur	- 349.58 - 379.77 161.42 244.01 - 500.54 - 230.53 93.00 × O-(C) ₂) + (1 re - Calculated	1.38 1.57 0.00 0.00 × C-(H)(O) ₃) = Residual 0.01	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL 64MCE/KIL C4H10O3 Reference
$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = $ Liquid ph. $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = $ 1,1'-Oxybi (2 × C _d - Gas phase $\Delta_{t}H^{\circ} = $ Liquid ph.	-362.00 204.01 427.27 ase -399.61 276.10 isethene; Eth-(H) ₂) + (1 × Literatu	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36 - 127.17 51.30 - 127.17 51.30 - 127.17 - 12.25 - 127.17 - 127.17	1.89 -3.30 21.64 -7.97 Divinyl ether < C _d -(O)(H)) d= Residual	69STU/WES 69STU/WES 75FEN/HAR 75FEN/HAR C4H6O Reference	Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ $C_p^\circ = S^\circ = $ $\Delta_t S^\circ = $ $\Delta_t G^\circ = $ $\ln K_t = $ Trimethoxym $(3 \times C - (H))$ Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$	348.20 348.20 378.20 161.42 244.01 ethane 3(C)) + (3 Literatur 545.00	- 349.58 - 379.77 161.42 244.01 - 500.54 - 230.53 93.00 × O-(C) ₂) + (1 re - Calculated - 545.01	1.38 1.57 0.00 0.00 × C-(H)(O) ₃) = Residual	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL 64MCE/KIL C4H10O3
$\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t = \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \Delta_t H^\circ = \frac{\Delta_t H^\circ = \Delta_t H^\circ = \Delta_$	-362.00 204.01 427.27 ase -399.61 276.10 isethene; Eth-(H) ₂) + (1 × Literatu	202.12 430.57 - 893.01 - 97.09 39.17 - 421.25 284.07 337.22 - 986.36 - 127.17 51.30 - 127.17 51.30 - 127.17 - 12.25 - 127.17 - 127.17	1.89 -3.30 21.64 -7.97 Divinyl ether < C _d -(O)(H)) i = Residual	69STU/WES 69STU/WES 75FEN/HAR 75FEN/HAR C4H60 Reference	Gas phase $\Delta_{t}H^{\circ} = -$ Liquid phase $\Delta_{t}H^{\circ} = -$ $C_{p}^{\circ} = $ $S^{\circ} = $ $\Delta_{t}S^{\circ} = $ $\ln K_{t} = $ Trimethoxym $(3 \times C - (H))$ Gas phase $\Delta_{t}H^{\circ} = -$ Liquid phase	348.20 -378.20 161.42 244.01 ethane 3(C)) + (3 Literatur	- 349.58 - 379.77 161.42 244.01 - 500.54 - 230.53 93.00 × O-(C) ₂) + (1 re - Calculated	1.38 1.57 0.00 0.00 × C-(H)(O) ₃) = Residual 0.01	Reference 69PIL/FLE 70BIR/SKI 64MCE/KIL 64MCE/KIL C4H10O Reference

TABLE 16. Ethers (53) - Continued

		×O-(C)₂)+(1:	× C-(H)(O) ₂ ($C_4H_{10}O_2$		•	Tetramethyl o $\times O-(C)_2$ + (1	rthocarbonate ×C-(O) ₄)	C ₅ H ₁₂ O
(17, 0223	•	e – Calculated :	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Das phase $\Delta_t H^\circ = -$	- 389.70	- 389.66	-0.04	69PIL/FLE	Gas phase Δ ₁ H° -	727.18	727.18	0.00	79WIB/SQU
Liquid phase $\Delta_t H^\circ = C_p^\circ =$	e 420.00	-418.09 170.36	-1.91	70BIR/SĶĪ	Liquid pha $\Delta_t H^\circ =$		-767.10	0.00	79WIB/SQU
	(C) + (2)	× O-(C) ₂) + (1	× C-(O) ₂ (C) ₂)	C ₅ H ₁₂ O ₂		H) ₃ (C)) + (1 H) ₂ (O)(C))	×C-(H)(O) ₂ (0 +(1×-CH ₃ cor	rr (tertiary))	
(2×-CH₃	corr (tertia		D :: 1	D 6		Literatu	re – Calculated	= Residual	Reference
Gas phase	Literatur	e – Calculated	= Residuai	Reference	Gas phase $\Delta_t H^{} =$	-453.59	- 455.46	1.87	68РІН/НЕІ
$\Delta_{\rm f}H^{\circ} = -$		- 429.96	5.65	79WIB/SQU	-	se -491.41	-489.69	- 1.72	68РІН/НЕІ
Liquid phase	e 459.48	-457.76	-1.72	79WIB/SQU	$C_p^{\circ} =$		237.64		
		Dioxaheptane		C ₃ H ₁₂ O ₂	1,2-Diethox (2×C-(1		× C-(H) ₂ (O)(C	C))+(2×O-(C	
Diethoxymet	thane; 3,5-1 () ₃ (C)) + (2 () ₂ (O) ₂)	Dioxaheptane × O-(C) ₂) + (2 re – Calculated			(2×C-(1	H)₃(C))+(4	×C-(H) ₂ (O)(C re Calculated		
Diethoxymei (2×C-(H (1×C-(H	thane; 3,5-1 () ₃ (C)) + (2 () ₂ (O) ₂)	\times O-(C) ₂)+(2		C))+		H)₃(C))+(4)2)
Diethoxymet $(2 \times C - (H \times C - (H \times C - (H \times C - (H \times C + (H \times C)))))))))))))))$	thane; 3,5-1 l) ₃ (C)) + (2 l) ₂ (O) ₂) Literatur - 414.80	× O-(C) ₂) + (2 re – Calculated	= Residual	C))+ Reference	$(2 \times C - (1))$ Gas phase $\Delta_t H^\circ =$	H)₃(C)) + (4 Literatur -408.19	re – Calculated – 418.96	= Residual	Reference
Diethoxymet $(2 \times C - (H + (1 \times C - (H + (H + (1 \times C - (H + (H + (1 \times C - (H + (H$	thane; 3,5-1 1) ₃ (C)) + (2 1) ₂ (O) ₂) Literatur - 414.80 se - 450.41	× O-(C) ₂) + (2 re - Calculated - 415.38 - 451.37 228.70 309.19 - 707.98 - 240.29 96.93	0.58 0.96	C))+ Reference 69MAN	Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ =$ $\Delta_t S^\circ = \Delta_t G^\circ =$ $\ln K_t =$ 3,5,7-Triox	H) ₃ (C)) + (4 Literatur - 408.19 se - 450.41 anonane H) ₃ (C)) + (2	- 418.96 169.86 - 460.08 256.06 350.52 - 802.96 - 220.68	= Residual 10.77 9.67	Reference 70KUZ/WAD 69MAN
Diethoxymet $(2 \times C - (H + (1 \times C - (H + (H$	thane; 3,5-1 l ₃ (C)) + (2 l) ₂ (O) ₂) Literatur - 414.80 se - 450.41 thoxyethane I) ₃ (C)) + (3	× O-(C) ₂) + (2 re - Calculated -415.38 -451.37 228.70 309.19 -707.98 -240.29 96.93	= Residual 0.58 0.96 × C-(O)₃(C))	C))+ Reference 69MAN 69MAN	Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ =$ $\Delta_t S^\circ = \Delta_t G^\circ =$ $\ln K_t =$ 3,5,7-Triox $(2 \times C - (1)$	H) ₃ (C)) + (4 Literatur - 408.19 se - 450.41 anonane H) ₃ (C)) + (2 H) ₂ (O) ₂)	- 418.96 169.86 - 460.08 256.06 350.52 - 802.96 - 220.68 89.02	= Residual 10.77 9.67	Reference 70KUZ/WAD 69MAN
Diethoxymei (2×C-(H) (1×C-(H) (1×C-(H) Gas phase $\Delta_t H^\circ = C_t^\circ = S_t^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t = 1,1,1-Trimet (4×C-(H) Gas phase$	thane; 3,5-1 l ₃ (C)) + (2 l) ₂ (O) ₂) Literatur - 414.80 se - 450.41 thoxyethane I) ₃ (C)) + (3	× O-(C) ₂) + (2 re - Calculated -415.38 -451.37 228.70 309.19 -707.98 -240.29 96.93 re × O-(C) ₂) + (1	= Residual 0.58 0.96 × C-(O)₃(C))	C))+ Reference 69MAN 69MAN C ₅ H ₁₂ O ₃	Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ =$ $\Delta_t S^\circ = \Delta_t G^\circ =$ $\ln K_t =$ 3,5,7-Triox $(2 \times C - (1)$	H) ₃ (C)) + (4 Literatur - 408.19 se - 450.41 anonane H) ₃ (C)) + (2 H) ₂ (O) ₂) Literatur	- 418.96 169.86 - 460.08 256.06 350.52 - 802.96 - 220.68 89.02 × C-(H) ₂ (O)(C	= Residual 10.77 9.67	Reference 70KUZ/WAD 69MAN C ₆ H ₁₄ O) ₂) +

C₆H₁₄O₃

TABLE 16. Ethers (53) - Continued

TABLE 16. Ethers (53) - Continued

3,5,7-Trioxanonane (Continued)
$(2 \times C - (H)_3(C)) + (2 \times C - (H)_2(O)(C)) + (3 \times O - (C)_2) +$
$(2\times C-(H)_2(O)_2)$

	Literatu	Reference		
Liquid ph	ıase			
$\Delta_t H^\circ =$	- 625.80	-625.09	-0.71	69MAN
$C_p^{\circ} = S^{\circ} =$		292.89		
s° =		359.82		
$\Delta_f S^\circ =$		-896.18		
$\Delta_f G^\circ =$		- 357.89		
$lnK_f =$		144.37		

1,3-Diethoxypropane	C7H16O2
$(2 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) + (4 \times C - (H)_2(O)(C)) +$	•
$(2\times O_{-}(C)_2)$	

Literatu	Literature – Calculated = Residual				
Gas phase $\Delta_t H^{\circ} = -436.18$	- 439.59	3.41	72MAN		
$C_p^{\circ} =$	192.75				
Liquid phase $\Delta_t H^\circ = -482.08$	-485.81	3.73	72MAN		
$C_p^{\circ} = S^{\circ} = S$	286.48 382.90				
$\Delta_t S^\circ = \Delta_t G^\circ =$	- 906.89 - 215.42				
$lnK_{\ell} =$	86.90				

2,2-Diethoxypropane $C_7H_{14}O_2$ $(4 \times C-(H)_3(C)) + (2 \times C-(H)_2(O)(C)) + (1 \times C-(O)_2(C)_2) +$ $(2 \times O-(C)_2) + (2 \times -CH_3 \text{ corr (quaternary))}$

	erature – Calculated	***	Reference
Gas phase $\Delta_t H^\circ = -506$.	.60 -500.36	- 6.24	62STE/DOR
Liquid phase $\Delta_t H^\circ = -538$.50 -533.78	-4.72	62STE/DOR
3,5,7,9-Tetraoxau (2×C-(H) ₃ (C) (3×C-(H) ₂ (O)	$+(2\times C-(H)_2(O)(C)$	C))+(4×O-((C7H16O4 C)2)+
Lite	erature – Calculated	= Residual	Reference

-742.66

1.66

69MAN

Gas phase $\Delta_t H^\circ = -741.00$

3,5,7,9-Tetraoxaundecane (Continued)	C7H16O4
$(2 \times C - (H)_2(C)) + (2 \times C - (H)_2(O)(C)) + (4 \times O - (C)_2) + (3 \times C - (H)_2(O)_2)$	
Literature - Calculated = Residual Ref	erence

	Literatu	Literature - Calculated = Residual					
Liquid phase							
$\Delta_t H^\circ =$	<i> 7</i> 94.60	-798.81	4.21	69MAN			
$C_p^{\circ} =$		357.08					
S° =		410.45					
$\Delta_f S^\circ =$		-1084.38					
$\Delta_f G^\circ =$		-475.50					
$lnK_f =$		191.81					

2-Methoxyethanol

C₃H₈O₂

 $(1 \times C - (H)_3(C)) + (1 \times O - (C)_2) + (1 \times O - (H)(C)) + (2 \times C - (H)_2(O)(C))$

	Literatur	Reference						
Gas phase								
$\Delta_i H^{\circ} =$		-368.81						
$C_p^{\circ} =$		103.09						
Liquid phas $\Delta_t H^\circ =$		-421.54						

2-Ethoxyethanol

 $C_4H_{10}O_2$

 $(1 \times C - (H)_3(C)) + (3 \times C - (H)_2(O)(C)) + (1 \times O - (C)_2) + (1 \times O - (H)(C))$

	Literatu	Reference		
Gas phase				
$\Delta_{\rm f} H^{\circ} =$		-401.71		
$C_p^{\circ} =$		123.42		
Liquid pha				
$\Delta_{\epsilon}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{\epsilon}S^{\circ} =$	210.80	-457.34 206.31 251.74 -629.12	4.49	73KUS/SUU
$C_p^{\circ} = S^{\circ} =$	210.80	206.31 251.74	4.49	73KUS/SUU

-			/FA\	_	
TABLE	16.	Ethers	(53)	_ C	ontinued

Diethylene (2×O-(F		C–(H)₂(O)(C	C))+(1×O-(C	C ₄ H ₁₀ O ₃	Triethylene (2×O-(×C-(H)₂(O)(C	C))+(2×O-(C	C ₆ H ₁₄ O ₆
	Literature -	- Calculated	= Residual	Reference	ce Literature – Calculated = Residual				Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 571.20	-551.68 136.18	- 19.52	37GAL/HIB	Gas phase $\Delta_t H^\circ = C_p^\circ =$	-725.00	- 718.90 195.38	-6.10	37GAL/HIB
Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ - \Delta_t G^\circ = \ln K_t =$	se 628.50 243.90	- 637.03 248.11 244.92 - 738.46 - 416.86 168.16	8.53 -4.21	37MOU/DOD 82ZAR	Liquid pha $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 804.20 333.70	-819.46 339.66 336.88 -1021.64 -514.86 207.69	15.26 5.96	37MOU/DOD 82ZAR
2-Propoxye (1×O-(1 (1×C-(1		C-(H)2(O)(C O-(C)2)	C))+(1×C-(H	$C_5H_{12}O_2$ $()_2(C)_2) +$	Tetraethyle (2×O-(H)(C))+(8	×C-(H)₂(O)(C		
	Literature ·	– Calculated	= Residual	Reference		Literatu ———	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$		-422.34 146.31			Gas phase $\Delta_i H^\circ = C_p^\circ =$	-883.00	- 886.12 254.58	3.12	37GAL/HIB
Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	se 241.60	-483.07 236.73 284.12 -733.05 -264.51 106.70	4.87	73KUS/SUU	Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	se - 981.70 428.80	- 1001.89 431.21 428.84 - 1304.83 - 612.86 247.22	20.19 - 2.41	37MOU/DOD 82ZAR
(2×C-(I	H)(C))+(2×0 H) ₃ (C))+ (1×	C-(H)(O)(C)) + (1 × O–(C C) ₂ (alcohols,p	C ₅ H ₁₂ O ₂ (2) ₂) + eroxides)) +		H) ₂ (O)(C)) lene oxide	$+(1 \times O-(C)_2)$ - rsc), $\sigma = 2$		C₂H₄O
(2×-CH	I itaratura	y)) Calculated	- Decidual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_l H^\circ = C_p^\circ =$	Literature	-441.69 148.78	- Residual	Reference	Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	- 52.60 48.28 242.42	-52.60 48.28 242.43 -132.72 -13.03 5.26	0.00 0.00 -0.01	65PEL/PIL 69STU/WES 69STU/WES
Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	238.80	-501.11 258.98 272.62 -744.55 -279.12 112.60	- 20.18	73KUS/SUU	Liquid phat $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se 77.61	-77.61 67.65 172.46 -202.68 -19.41 7.83	0.00	49GIA/GOR

.60 0.00	Reference 52GUT/SCO
	52GUT/SCO
	52GUT/SCO
.60 0.00	
.60 0.00	
.60 0.00	
	52GUT/SCO
$(C)(C) + (2 \times C - (H)_2(C))$	C ₄ H ₈ O
= 2	12) .
ulated = Residual	Reference
.20 0.00	65PEL/PIL
.25 0.00	86CHA/HAL
.41 0.00	86CHA/HAL
.36	
.16	
.74	· .
	57SKU/STR
	85WIL/CHA
	85WIL/CHA
.02	
.01	
.89	
	
N	C ₄ H ₈ O ₂
	J))+
oxane rsc)	
ulated = Residual	Reference
.59 -0.01	82BYS/MAN
	
	82BYS/MAN
.90 0.00	82BYS/MAN
	AND I WITH THE
	1.25 0.00 1.41 0.00 1.36 1.16 1.74 1.19 0.00 1.90 0.00 1.90 0.00 1.90 0.00 1.90 0.00 1.90 0.00 1.89 1.19 0.00 1.90 0.00 1.90 0.00 1.90 0.00 1.90 0.00 1.90 0.00 1.89 1.10 0.00 1.89 0.00 1.80 0.00 1.8

		(H) ₂ (O)(C))+			(3 × C _B -($H)(C_B)_2)$			$(C_B)_2) +$
	Literature	- Calculated =	Residual	Reference		Literatui	e – Calculated	= Residual	Reference
jas phase									
$\Delta_i H^\circ = -$	_315 30	-315.29	-0.01	82BYS/MAN	Liquid phas	ge.			
							117.07	2.47	TENTAL AD
$C_p^{\circ} =$	94.06	94.06	0.00	69STU/WES	-	-114.80	-117.27	2.47	75FEN/HAR
<i>s</i> ° =	299.78	299.78	0.00	69STU/WES	$C_p^{\circ} =$	199.00	197.69	1.31	75FEN/HAR
$\Delta_{\mathbf{f}}S^{\circ} =$		- 450.51							
$\Delta_t G^\circ =$		- 180.97							
$lnK_f =$		73.00							
1		, , , , ,			Ethovybenz	ene: Ethyl :	ohenyl ether; P	henetale	C ₈ H ₁₀
					(1×C-(H	(C) + (1	× C-(H) ₂ (O)(C	C))+(1×O-(0	
Liquid phase					$(1 \times C_{B}-($	$O((C_B)_2) +$	$(5 \times C_B - (H)(C_F))$	3)2)	
-	- 355.10	- 355.10	0.00	82BYS/MAN					
$C_p^{\circ} =$	153.60	153.60	0.00	85WIL/CHA		Literatur	e - Calculated	= Residual	Reference
S° =	270.20	270.20	0.00	85WIL/CHA		-			
$\Delta_{f}S^{\circ} =$		- 480.09							
Δρ = Δ _t G° =		- 480.09 - 212.02			Gas phase				
-					•	101.20	100.44	1.04	APTITUTE
$lnK_f =$		85.53			$\Delta_{\rm f}H^{\circ} =$	- 101.60	- 103.41	1.81	75FEN/HAR
							· · · · · · · · · · · · · · · · · · ·		
Oxane; Tetra	ahydropyrai	n.		C ₅ H ₁₀ O	Liquid phas	se			
(1×O-(C	$(2)_2$) + $(2 \times C$ -	$-(H)_2(O)(C)) +$	$(3 \times C - (H)_2)$	C) ₂) +	$\Delta_{\rm f} H^{\circ} =$	- 152.60	-153.07	0.47	75FEN/HAR
	ydropyran		. , ,-,	• • .	$C_{p}^{\circ} =$	228.50	231.33	-2.83	75FEN/HAR
(·, _F , ·								
	Literature	- Calculated =	Residual	Reference					
					1. Mathawy	3. mathylhar	zene; Methyl t	alul athar	C ₈ H ₁₀
C b					•	•		•	
Gas phase	000.40	000.40	0.00	CEDEL DIL			\times O-(C)(C _B)) +		
$\Delta_i H^\circ = -$	- 223.40	- 223.40	0.00	65PEL/PIL	$(1 \times C_B - ($	$C)(C_B)_2)+($	$(4 \times C_B - (H)(C_B))$	$)_2) + (1 \times meta)$	corr)
						Literatur	e – Calculated	= Residual	Reference
Liquid phas									
$\Delta_{f}H^{\circ} = \cdot$	- 258.30	-258.30	0.00	58CAS/FLE2					
$C_p^{\circ} =$	140.60	140.59	0.01	76CON/GIN	Gas phase				
					$\Delta_t H^{\circ} =$	- 104.10	- 103.57	- 0.53	70COX/PIL
1,3-Dioxepa	me			$C_5H_{10}O_2$					
		(H)-(O)-) + (2	۸ (- (H) (O)		Liquid phas				
		$-(H)_2(O)_2) + (2)_2$		(C)) T			150.00	1 70	41D 4 D
(2×C-(H	$(1)_2(C)_2 + (1)_2$	×1,3-dioxepane	e rsc)			- 155.60	153.88	- 1.72	41BAD
					$C_p^{\circ} =$		221.59		
	Literature	e – Calculated =	Residual	Reference					
Gas phase					1,2-Dimetho	oxybenzene			C ₈ H ₁₀ C
	- 346.60	-346.60	0.00	70COX/PIL	•	•	\times O-(C)(C _B)) +	- (2 × C _R -(O)(
							(1×ortho corr)		/•/
					, -5 (- 4
iquid phas		007.60	0.00	EGOVI L'OTTO		Literatur	e – Calculated :	= Kesidual	Reference
$\Delta_i H^{\circ} =$	-387.60	-387.60	0.00	57SKU/STR					
	167.40	167.38	0.02	76CON/GIN					
$C_p^{\circ} =$			·	· · · · · · · · · · · · · · · · · · ·	Gas phase				
C _p =					$\Delta_{\epsilon}H^{\circ} =$	- 223.38	- 222.62	- 0.76	58CAS/FLE3
<i>C</i> _p =	*								
			Amirale	0110					
Methoxyben		yl phenyl ether;		C ₇ H ₈ O	.,				
Methoxyben		yl phenyl ether; ×O-(C)(C _B))+			Liquid phas				
Methoxyben	I)₃(C))+(1					se 290.30	- 280.24	- 10.06	58CAS/FLE3
Methoxyben (1×C-(H	I)₃(C))+(1				$\Delta_t H^\circ =$		280.24 262.80	- 10.06	58CAS/FLE3
Methoxyben (1×C-(H	$(C_B)_3$ $(C_B)_2$ $(C_B)_2$		$(1 \times C_B - (O))$					-10.06	58CAS/FLE3
Methoxyben (1×C-(H	$(C_B)_3$ $(C_B)_2$ $(C_B)_2$	× O-(С)(С _в)) +	$(1 \times C_B - (O))$	$(C_B)_2) +$	$\Delta_t H^\circ =$			- 10.06	58CAS/FLE3
Methoxyben (1 × C-(H (5 × C _B -(l	$(C_B)_3$ $(C_B)_2$ $(C_B)_2$	× O-(С)(С _в)) +	$(1 \times C_B - (O))$	$(C_B)_2) +$	$\Delta_t H^\circ =$			- 10.06	58CAS/FLE3
Methoxyben (1 × C-(H (5 × C _B -(l	I) ₃ (C))+(12 H)(C _B) ₂) Literature	\times O-(C)(C _B))+ $=$ - Calculated =	(1×C _B -(O)((C _B) ₂) + Reference	$\Delta_t H^\circ =$			- 10.06	58CAS/FLE3
Methoxyben (1 × C-(H (5 × C _B -(l	$(C_B)_3$ $(C_B)_2$ $(C_B)_2$	× O-(С)(С _в)) +	$(1 \times C_B - (O))$	$(C_B)_2) +$	$\Delta_t H^\circ =$			- 10.06	58CAS/FLE3

Table 17. Aldehydes (16)

	TABLE 16. Ethers (53) — Continued			TABLE 17. Aldehydes (16)					
Diphenyl o	xide	phenyl ether;	' _B)₂)+(1×O-	C ₁₂ H ₁₀ O	Methanal;		y de naldehyde), σ =	= 2	CH₂C
(2011.08 (Literature – Calculated = Residual		Reference	Literature – Calculated = Residual			= Residual	Reference	
Gas phase Δ _t H° =	52.00	50.94	1.06	72MOR2	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ $	-108.60 35.40 218.78	-108.60 35.40 218.78 -20.06 -102.62	0.00 0.00 0.00	70FLE/PIL 69STU/WES 69STU/WES
$\Delta_f H^\circ = S^\circ = \Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$	-14.90	-14.89 290.83 -533.43 144.15 -58.15	-0.01	51FUR/GIN	$\ln K_{\ell} = \frac{1}{2}$ Ethanal; Ac	-	41.40 ×CO-(H)(C)	$\alpha = 3$	C₂H₄0
Solid phase	······································		· · · · · · · · · · · · · · · · · · ·		(1 × C (1		re – Calculated		Reference
$\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-32.10 216.56 233.93	-28.90 216.62 233.82 -590.44 147.14 -59.35	-3.20 -0.06 0.11	51FUR/GIN 51FUR/GIN 51FUR/GIN	Gas phase $\Delta_t H^* = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 166.10 54.64 264.22	- 166.65 54.73 265.22 - 109.93 - 133.87 54.00	0.55 - 0.09 - 1.00	38DOL/GRE 69STU/WES 69STU/WES
					Liquid phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f = $	99.05 117.30	- 190.03 101.58 176.85 - 198.29 - 130.91 52.81	-1.77 -12.53 -59.55	49COL/DEV 88LEB/VAS 88LEB/VAS
					Ethanedial; (2×CO~	Glyoxal (H)(CO))			C ₂ H ₂ O ₂
						Literatur	re – Calculated	= Residual	Reference
					Gas phase $\Delta_t H^\circ =$	- 211.96	-211.96	0.00	70FLE/PIL
					Propanal; F			(C))+(1×CO	C_3H_6O -(H)(C)), $\sigma = 3$
						Literatur	e – Calculated	= Residual	Reference
					Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	189.40 78.66 304.72	- 188.49 79.42 304.80 - 206.66 - 126.87 51.18	0.91 0.76 0.08	67BUC/COX 69STU/WES 69STU/WES

TABLE 17. Aldehydes (16) - Continued

TABLE 17.	Aldehydes	(16) -	Continued
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		nyde (Continue × C–(H)2(CO)(C_3H_6O -(H)(C)), $\sigma = 3$			\times C-(H) ₂ (C) ₂) + (1 × C-(H) ₂	C ₅ H ₁₀ ((CO)(C))+
	Literatur	e – Calculated :	= Residual	Reference	(1×00		re – Calculatec	l = Residual	Reference
iquid phas	e							 	
	-215.30	-214.17	-1.13	67BUC/COX	Gas phase				
$C_p^{\circ} =$	159.10	130.87	28.23	77KOR/VAS	$\Delta_{\mathbf{f}}H^{\circ} =$	-228.50	-229.75	1.25	70CON
S° =	212.90	216.72	-3.82	77KOR/VAS	$C_p^{\circ} =$	125.35	125.20	0.15	69STU/WES
$\Delta_{\mathbf{f}}S^{\circ} =$		- 294.73			S° =	382.96	383.12	-0.16	69STU/WES
$\Delta_{\rm f}G^{\circ} =$		-126.29			$\Delta_{\mathbf{f}}S^{\circ} =$		-400.96		
$lnK_f =$		50.95			$\Delta_f G^\circ =$		-110.20		
					$lnK_f =$		44.46		
rans-2-But	enal; Croto	naldehvde		C ₄ H ₆ O	Liquid pha	se			
	-	× C _d -(H)(C)) +	- (1 × C _d (H)($\Delta_t H^\circ =$	-267.30	-265.63	-1.67	70CON
(1×CO-		- \ /\ //		•	$C_p^{\circ} =$	174.39	191.71	-17.32	84VAS/PET
•					S° =	273.59	281.48	-7.89	84VAS/PET
	Literatur	e - Calculated	= Residual	Reference	$\Delta_t S^{\circ} =$		-502.60		
····					$\Delta_{\rm f}G^{\circ} =$		-115.78		
Gas phase					$lnK_f =$		46.71 		
	100.60	- 100.60	0.00	38DOL/GRE					
					Hexanal; H	exaldehyde			C ₆ H ₁₂ C
Liquid phas Δ _f H° =	se 144.10	-143.00	-1.10	60ТЈЕ	(1×C-(I (1×CO-	H) ₃ (C)) + (3 -(H)(C)), σ) + (1 × C-(H) ₂ (
			-			Literatu	re – Calculated	l = Residual	Reference
	ıtyraldehyd		-	C ₄ H ₈ O		Literatui	re – Calculated	l = Residual	Reference
(1 × C-(F	(C) + (1	\times C-(H) ₂ (C) ₂)	+ (1×C-(H) ₂		Gas phase	Literatui		l = Residual	Reference
(1×C-(F		\times C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂		$\Delta_{\rm f}H^{\circ} =$	7mm 1 (///m A A PAN)	-250.38		
(1 × C-(F	H) ₃ (C)) + (1 (H)(C)), σ	$\times C - (H)_2(C)_2$ = 3		(CO)(C))+	$\Delta_t H^{\circ} = C_p^{\circ} =$	148.24	-250.38 148.09	0.15	69STU/WES
(1 × C-(F	H) ₃ (C)) + (1 (H)(C)), σ	\times C-(H) ₂ (C) ₂)			$\Delta_t H^{\circ} = C_{\rho}^{\circ} = S^{\circ} =$	7mm 1 (///m A A PAN)	-250.38 148.09 422.28		
(1 × C-(F	H) ₃ (C)) + (1 (H)(C)), σ	$\times C - (H)_2(C)_2$ = 3		(CO)(C))+	$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = C_p^{\circ} = C_$	148.24	-250.38 148.09 422.28 -498.11	0.15	69STU/WES
(1×C-(I (1×CO-	H) ₃ (C)) + (1 (H)(C)), σ	$\times C - (H)_2(C)_2$ = 3		(CO)(C))+	$\Delta_t H^{\circ} = C_{\rho}^{\circ} = S^{\circ} =$	148.24	-250.38 148.09 422.28	0.15	69STU/WES
(1×C-(I (1×CO-	H) ₃ (C)) + (1 (H)(C)), σ	$\times C-(H)_2(C)_2$ = 3 re - Calculated - 209.12		(CO)(C))+	$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = S^{\circ} $	148.24	- 250.38 148.09 422.28 - 498.11 - 101.87	0.15	69STU/WES
$(1 \times C - (1 \times CO - 1 \times CO - $	H ₃ (C)) + (1 (H)(C)), σ Literatur -204.70 102.59	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31	= Residual 4.42 0.28	(CO)(C))+ Reference	$\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = S^{\circ} $	148.24	- 250.38 148.09 422.28 - 498.11 - 101.87	0.15	69STU/WES
$(1 \times C - (I \times CO - I) \times CO - I)$ Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = I$	$H_{3}(C)$) + (1 (H)(C)), σ Literatur -204.70	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96	= Residual	(CO)(C))+ Reference 79SUN/SVE	$\Delta_{\ell}H^{\circ} =$ $C_{\rho}^{\circ} =$ $S^{\circ} =$ $\Delta_{\ell}S^{\circ} =$ $\Delta_{\ell}G^{\circ} =$ $\ln K_{\ell} =$ Liquid pha	148.24 422.88	-250.38 148.09 422.28 -498.11 -101.87 41.09	0.15	69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	H ₃ (C)) + (1 (H)(C)), σ Literatur -204.70 102.59	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81	= Residual 4.42 0.28	(CO)(C))+ Reference 79SUN/SVE 69STU/WES	$\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phat $\Delta_t H^\circ =$	148.24 422.88	-250.38 148.09 422.28 -498.11 -101.87 41.09	0.15 0.60	69STU/WES 69STU/WES
$(1 \times C - (1 \times C) - (1 \times C) - (1 \times C)$ Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = C_{p}^{\circ} = C_{p$	H ₃ (C)) + (1 (H)(C)), σ Literatur -204.70 102.59	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54	= Residual 4.42 0.28	(CO)(C))+ Reference 79SUN/SVE 69STU/WES	$\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phat $\Delta_t H^\circ =$ $C_p^\circ =$	148.24 422.88	-250.38 148.09 422.28 -498.11 -101.87 41.09	0.15 0.60	69STU/WES 69STU/WES 91VAS/BYK
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	H ₃ (C)) + (1 (H)(C)), σ Literatur -204.70 102.59	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81	= Residual 4.42 0.28	(CO)(C))+ Reference 79SUN/SVE 69STU/WES	$\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phat $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$	148.24 422.88	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86	0.15 0.60	69STU/WES 69STU/WES
$(1 \times C - (I \times C) - (I \times C) - (I \times C)$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = I$	H ₃ (C)) + (1 (H)(C)), σ Literatur -204.70 102.59	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54	= Residual 4.42 0.28	(CO)(C))+ Reference 79SUN/SVE 69STU/WES	$\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid phat $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \frac{1}{2}$	148.24 422.88	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53	0.15 0.60	69STU/WES 69STU/WES 91VAS/BYK
$(1 \times C - (I \times CO - I) \times CO - I)$ Gas phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t = InK_t$	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54	= Residual 4.42 0.28	(CO)(C))+ Reference 79SUN/SVE 69STU/WES	$\Delta_t H^\circ =$ $C^\circ_\rho =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phat $\Delta_t H^\circ =$ $C^\circ_\rho =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	148.24 422.88	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53 -110.52	0.15 0.60	69STU/WES 69STU/WES 91VAS/BYK
$(1 \times C - (I \times C) - (1 \times C) - (1 \times C)$ Gas phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = 1$ Liquid phase	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54 47.82	= Residual 4.42 0.28 0.97	Reference 79SUN/SVE 69STU/WES 69STU/WES	$\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Liquid phat $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \frac{1}{2}$	148.24 422.88	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53	0.15 0.60	69STU/WES 69STU/WES 91VAS/BYK
$(1 \times C - (H + C) - (1 \times C) - (1 \times C) - (1 \times C)$ Gas phase $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t G^\circ = InK_t $	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54 47.82	= Residual 4.42 0.28 0.97	(CO)(C))+ Reference 79SUN/SVE 69STU/WES 69STU/WES	$\Delta_t H^\circ =$ $C^\circ_\rho =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phat $\Delta_t H^\circ =$ $C^\circ_\rho =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	148.24 422.88	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53 -110.52	0.15 0.60	69STU/WES 69STU/WES 91VAS/BYK
$(1 \times C - (I \times CO - I) \times CO - I)$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t = InK_t$	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54 47.82 - 239.90 161.29	= Residual 4.42 0.28 0.97 0.50 3.41	Reference 79SUN/SVE 69STU/WES 69STU/WES 79SUN/SVE 89VAS/LEB	$\Delta_t H^\circ =$ $C^\circ_\rho =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phat $\Delta_t H^\circ =$ $C^\circ_\rho =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	148.24 422.88	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53 -110.52	0.15 0.60	69STU/WES 69STU/WES 91VAS/BYK
$(1 \times C - (H \cap I) \times CO - I)$ Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = InK_t = I$ Liquid phase $\Delta_t H^\circ = C_p^\circ = InK_t = I$	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54 47.82	= Residual 4.42 0.28 0.97	(CO)(C))+ Reference 79SUN/SVE 69STU/WES 69STU/WES	$\Delta_t H^\circ =$ $C^\circ_\rho =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phat $\Delta_t H^\circ =$ $C^\circ_\rho =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	148.24 422.88 se 210.40 280.30	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53 -110.52 44.58	0.15 0.60	69STU/WES 69STU/WES 91VAS/BYK
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \ln K_{f} = $ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} $	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54 47.82 - 239.90 161.29 249.10	= Residual 4.42 0.28 0.97 0.50 3.41	Reference 79SUN/SVE 69STU/WES 69STU/WES 79SUN/SVE 89VAS/LEB	$\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid pha: $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	148.24 422.88 se 210.40 280.30	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53 -110.52 44.58	0.15 0.60	69STU/WES 69STU/WES 91VAS/BYK 91VAS/BYK
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \ln K_f = $ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = S_t H^\circ = S^\circ = S^$	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54 47.82 - 239.90 161.29 249.10 - 398.67	= Residual 4.42 0.28 0.97 0.50 3.41	Reference 79SUN/SVE 69STU/WES 69STU/WES 79SUN/SVE 89VAS/LEB	$\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phat $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t =$ Heptanal; 1 $(1 \times C - (H^\circ)^\circ = S^\circ = L^\circ + L^\circ +$	148.24 422.88 se 210.40 280.30	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53 -110.52 44.58	0.15 0.60 -11.73 -33.56	69STU/WES 69STU/WES 91VAS/BYK 91VAS/BYK
Gas phase $\Delta_{t}H^{\circ} = C^{\circ}_{t} = S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}_{t}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}_{t}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}_{t}} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}_{t}} = \frac{\Delta_{t}S^{\circ}}{\Delta_{t}G^{\circ}} = \frac{\Delta_{t}S^{\circ}}{S^{\circ}_{t}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}_{t}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}_{t}} = \frac{\Delta_{t}G^{\circ}}{S^{\circ}_{t}} = \frac{\Delta_{t}G^{\circ}_{t}}{S^{\circ}_{t}} $	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54 47.82 - 239.90 161.29 249.10 - 398.67 - 121.04	= Residual 4.42 0.28 0.97 0.50 3.41	Reference 79SUN/SVE 69STU/WES 69STU/WES 79SUN/SVE 89VAS/LEB	$\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phat $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t =$ Heptanal; 1 $(1 \times C - (H^\circ)^\circ = S^\circ = L^\circ + L^\circ +$	148.24 422.88 se 210.40 280.30 Heptaldehyd H ₃ (C)) + (4 (H)(C)), σ	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53 -110.52 44.58	0.15 0.60 -11.73 -33.56	69STU/WES 69STU/WES 91VAS/BYK 91VAS/BYK
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ$	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54 47.82 - 239.90 161.29 249.10 - 398.67 - 121.04	= Residual 4.42 0.28 0.97 0.50 3.41	Reference 79SUN/SVE 69STU/WES 69STU/WES 79SUN/SVE 89VAS/LEB	$\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phat $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t =$ Heptanal; 1 $(1 \times C - (H^\circ)^\circ = S^\circ = L^\circ + L^\circ +$	148.24 422.88 se 210.40 280.30 Heptaldehyd H ₃ (C)) + (4 (H)(C)), σ	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53 -110.52 44.58	0.15 0.60 -11.73 -33.56	69STU/WES 69STU/WES 91VAS/BYK 91VAS/BYK C ₇ H ₁₄ C
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = $ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{$	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54 47.82 - 239.90 161.29 249.10 - 398.67 - 121.04	= Residual 4.42 0.28 0.97 0.50 3.41	Reference 79SUN/SVE 69STU/WES 69STU/WES 79SUN/SVE 89VAS/LEB	$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \Delta_t H^\circ = C_p^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t G^\circ = \ln K_t = \frac{\Delta_t G^\circ = L^\circ C_t G^\circ = L^\circ C_t G^\circ = L^\circ C_t G^\circ = \frac{L^\circ C_t G^\circ = L^\circ C_t G^\circ = L^\circ C_t G^\circ = \frac{L^\circ C_t G^\circ = L^\circ C_t G^\circ = L^\circ C_t G^\circ = \frac{L^\circ C_t G^\circ = L^\circ C_t G^\circ = L^\circ C_t G^\circ = \frac{L^\circ C_t G^\circ C_t G^\circ G^\circ = L^\circ C_t G^\circ G^\circ = L^\circ C_t G^\circ G^\circ = \frac{L^\circ C_t G^\circ G^\circ G^\circ G^\circ G^\circ G^\circ G^\circ G^\circ G^\circ G^\circ$	148.24 422.88 se 210.40 280.30 Heptaldehyd H ₃ (C)) + (4 (H)(C)), σ	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53 -110.52 44.58	0.15 0.60 -11.73 -33.56	69STU/WES 69STU/WES 91VAS/BYK 91VAS/BYK C ₇ H ₁₄ C
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = $ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{$	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54 47.82 - 239.90 161.29 249.10 - 398.67 - 121.04	= Residual 4.42 0.28 0.97 0.50 3.41	Reference 79SUN/SVE 69STU/WES 69STU/WES 79SUN/SVE 89VAS/LEB	$\Delta_t H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t S^{\circ} = \ln K_t = \frac{\Delta_t H^{\circ}}{C_{\rho}^{\circ}} = \frac{\Delta_t H^{\circ}}{C_{\rho}^{\circ}} = \frac{\Delta_t S^{\circ}}{L_t G^{\circ}} = \ln K_t = \frac{(1 \times C - (1 \times C - C))}{C_t G^{\circ}}$ Gas phase	148.24 422.88 se 210.40 280.30 Heptaldehyddil) ₃ (C)) + (4 (H)(C)), σ Literatur	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53 -110.52 44.58	0.15 0.60 -11.73 -33.56 +(1×C-(H) ₂ (69STU/WES 69STU/WES 91VAS/BYK 91VAS/BYK (CO)(C)) +
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ$	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54 47.82 - 239.90 161.29 249.10 - 398.67 - 121.04	= Residual 4.42 0.28 0.97 0.50 3.41	Reference 79SUN/SVE 69STU/WES 69STU/WES 79SUN/SVE 89VAS/LEB	$\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phate $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t =$ Heptanal; I $(1 \times C - (K_t) + (K_t$	148.24 422.88 se 210.40 280.30 Heptaldehyd H ₃ (C)) + (4 (H)(C)), σ Literatur	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53 -110.52 44.58	0.15 0.60 -11.73 -33.56 +(1×C-(H) ₂ (69STU/WES 69STU/WES 91VAS/BYK 91VAS/BYK (CO)(C)) + Reference
$(1 \times C - (I \times C) - (I \times $	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54 47.82 - 239.90 161.29 249.10 - 398.67 - 121.04	= Residual 4.42 0.28 0.97 0.50 3.41	Reference 79SUN/SVE 69STU/WES 69STU/WES 79SUN/SVE 89VAS/LEB	$\Delta_{t}H^{\circ} =$ $C_{p}^{\circ} =$ $S^{\circ} =$ $\Delta_{t}S^{\circ} =$ $\Delta_{t}G^{\circ} =$ $\ln K_{t} =$ Liquid phat $\Delta_{t}H^{\circ} =$ $C_{p}^{\circ} =$ $S^{\circ} =$ $\Delta_{t}S^{\circ} =$ $\ln K_{t} =$ Heptanal; I $(1 \times C - (H \times CO - H \times C))$ Gas phase $\Delta_{t}H^{\circ} =$ $C_{p}^{\circ} =$ $S^{\circ} =$ $\Delta_{t}S^{\circ} =$ $\Delta_{t}S^{\circ} =$ $\Delta_{t}S^{\circ} =$	148.24 422.88 se 210.40 280.30 Heptaldehyd 1) ₃ (C)) + (4 (H)(C)), σ Literatur - 263.80 171.08	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53 -110.52 44.58 	0.15 0.60 - 11.73 - 33.56 + (1 × C-(H) ₂ (69STU/WES 69STU/WES 91VAS/BYK 91VAS/BYK 91VAS/BYK C7H14O (CO)(C))+ Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \Delta_t H^\circ = C_p^\circ = \Delta_t G^\circ = \frac{\Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \frac{\Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \frac{\Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \frac{\Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \frac{\Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \frac{\Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \frac{\Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \frac{\Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \frac{\Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \Delta_t G^\circ = \frac{\Delta_t G^\circ = \Delta_t G^\circ = \frac{\Delta_t G^\circ = \Delta_t G^$	H ₃ (C)) + (1 (H)(C)), σ Literatur - 204.70 102.59 344.93	× C-(H) ₂ (C) ₂) = 3 re - Calculated - 209.12 102.31 343.96 - 303.81 - 118.54 47.82 - 239.90 161.29 249.10 - 398.67 - 121.04	= Residual 4.42 0.28 0.97 0.50 3.41	Reference 79SUN/SVE 69STU/WES 69STU/WES 79SUN/SVE 89VAS/LEB	$\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phate $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t =$ Heptanal; I $(1 \times C - (K_t) + (K_t$	148.24 422.88 se 210.40 280.30 Heptaldehyd 1) ₃ (C)) + (4 (H)(C)), σ Literatur - 263.80 171.08	-250.38 148.09 422.28 -498.11 -101.87 41.09 -291.36 222.13 313.86 -606.53 -110.52 44.58 	0.15 0.60 - 11.73 - 33.56 + (1 × C-(H) ₂ (69STU/WES 69STU/WES 91VAS/BYK 91VAS/BYK 91VAS/BYK (CO)(C)) + Reference 70COX/PIL 69STU/WES

TABLE 17. Aldehydes (16) - Continued

(1×C-(H		e (Continued) \times C-(H) ₂ (C) ₂) - = 3	+ (1×C-(H)₂(C ₇ H ₁₄ O (CO)(C))+			$ \times C - (H)_2(C)_2 $ $ = 3 $	+ (1 × C-(H) ₂	C ₁₀ H ₂₀ O (CO)(C)) +
	Literatur	e – Calculated :	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ - \Delta_t G^\circ = \ln K_t =$	-311.50 230.15 335.43	-317.09 252.55 346.24 -710.46 -105.27 42.46	5.59 - 22.40 - 10.81	60NIC 84VAS/PET 84VAS/PET	Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	239.70 578.56	- 332.90 239.65 578.92 - 886.72 - 68.53 27.64	0.05 0.36	69STU/WES 69STU/WES
	I) ₃ (C))+(5 (H)(C)), σ	$\times C-(H)_2(C)_2)$ = 3 $e - Calculated$		C ₈ H ₁₆ O (CO)(C))+ Reference	Liquid pha $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	319.67 429.46	-394.28 343.81 443.38 -1022.25 -89.50 36.10	- 24.14 - 13.92	84VAS/PET 84VAS/PET
Gas phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t^\circ =$	193.97 500.66	-291.64 193.87 500.60 -692.41 -85.20 34.37	0.10 0.06	69STU/WES 69STU/WES	(2×C-(I	$(H)_5(C)$) + (1) $(G)_3$ corr (terti	butyraldehyde × C-(H)(CO)(iary)) re – Calculated		C₄H₅O ⊢(H)(C)) + Reference
Liquid phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = S^\circ $	259.58 365.45	-342.82 282.97 378.62 -814.39 -100.01 40.34	-23.39 -13.17	84VAS/PET 84VAS/PET	Gas phase $\Delta_l H^\circ =$ Liquid pha $\Delta_l H^\circ =$ $C_l^\circ =$	-215.80 se -247.30	-213.68 -245.89 155.47	-2.12 -1.41	75CON 75CON
	•	\times C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂	C ₂ H ₁₈ O (CO)(C))+	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} =$	re 	235.63 -412.14 -123.01 49.62		
	Literatur	re – Calculated	= Residual	Reference	2-Ethylhex: (2×C-(I (1×CO-	$H)_3(C)) + (4$	× C-(H) ₂ (C) ₂)	+ (1 × C-(H)(C ₈ H ₁₆ O
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	216.81 539.61	-312.27 216.76 539.76 -789.56 -76.86 31.01	0.05 - 0.15	69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ =$		e – Calculated	= Residual - 7.94	Reference 70COX/PIL
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	290.26 396.92	-368.55 313.39 411.00 -918.32 -94.75 38.22	-23.13 -14.08	84VAS/PET 84VAS/PET	Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	se 348.50	- 344.45 277.15 365.15 - 827.86 - 97.62 39.38	4.05	60TJE

TABLE 17. Aldehydes (16) - Continued

TABLE 18. Ketones (42)

		(1×C _B -(CO)(C (1×Furan rsc)	$(C_B)_2$) + $(1 \times O$	$ C_5H_4O_2 - (C_B)_2) +$			Dimethyl ketono (1×CO-(C) ₂),		C ₃ H ₆ (
		re – Calculated =	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase Δ _i H° =	- 151.04	-154.26	3.22	75KUD/KUD	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	-217.50 74.89 294.93	-217.19 74.89 294.92	0.31 0.00 0.01	65BUC/HER 69STU/WES 69STU/WES
Liquid phas Δ _t H° =	se -201.60	-198.38	-3.22	29LAN/BAY	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-216.54 -152.63 61.57		
Benzaldehy	de			C₁H₄O	Liquid pho $\Delta_t H^\circ =$	se 248.10	- 247.98	-0.12	57PEN/KOB
(5×C _B -((1 × C _B -(CO)(C		$C-(H)(C_B)$, $\sigma = 2$ Reference	$C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} $	124.68 200.41	125.93 200.41 - 311.04 - 155.24	-1.25 0.00	29KEL3 29KEL3
Gas phase $\Delta_t H^\circ =$	-36.80	- 36.80	0.00	75AMB/CON	$\ln K_{\rm f} =$		62.62		· · · · · · · · · · · · · · · · · · ·
Liquid pha		04.00		75.13.4D.(CO.).	Butanone; 1 (2×C-(F		vi ketone ×CO-(C) ₂)+((1×C-(H)₂(C	C_4H_8 O)(C)), $\sigma = 9$
$\Delta_t H^\circ = C_p^\circ =$	- 86.82 172.00	- 86.82 172.01	0.00 -0.01	75AMB/CON 75AMB/CON		Literatu	re – Calculated	= Residual	Reference
			·		Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\ln K_f =$	-238.90 102.88 338.11	- 239.03 99.58 340.26 - 307.50 - 147.35 59.44	0.13 3.30 -2.15	79SUN/SVE 69STU/WES 69STU/WES
					Liquid phat $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se - 273.20 158.70 239.00	- 272.12 155.22 240.28 - 407.49 - 150.63 60.76	-1.08 3.48 -1.28	79SUN/SVE 68AND/COU 68AND/COU
					(2×C-(I		oropyl ketone ×C-(H) ₂ (C) ₂) 18	+ (1 × C-(H) ₂ (C ₅ H ₁₀ (CO)(C)) +
						Literatu	re – Calculated	= Residual	Reference
					Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	-259.05 120.96 376.18	- 259.66 122.47 373.66 - 410.42 - 137.29 55.38	0.61 -1.51 2.52	70HAR/HEA 69STU/WES 69STU/WES

TABLE 18. Ketones (42) - Continued

TABLE 18. Ketones (42) - Continued

(2×C-(H		ropyl ketone (0 × C-(H) ₂ (C) ₂) 18		(CO)(C) +	(2×C-(I	e; Ethyl pro H)3(C))+(1 H)2(C)2), σ	\times CO-(C) ₂)+	(2×C-(H)₂(C	C ₆ H ₁₂ (O)(C)) +
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid phas	sc				Gas phase				
$\Delta_{f}H^{\circ} =$	-297.29	- 297.85	0.56	70HAR/HEA	$\Delta_t H^\circ =$	-278.25	-281.50	3.25	70HAR/HEA
$C_p^{\circ} =$	184.20	185.64	- 1.44	68AND/COU	$C_p^{\circ} =$		147.16		
S° =	274.10	272.66	1.44	68AND/COU	s° =		413.24		
$\Delta_f S^{\circ}$ —		-511.42			$\Delta_{t}S^{\circ}$ –		-507.15		
$\Delta_{\mathbf{f}}G^{\circ} =$		- 145.37			$\Delta_{\rm f}G^{\circ} =$		-130.29		
$lnK_f =$		58.64			$lnK_f =$		52.56		~~
					Liquid pha				
3-Pentanon			(C)) + (1 × CC	$C_5H_{10}O$	$\Delta_{\rm f}H^{\circ} =$	-320.13	-321.99	1.86	70HAR/HEA
(2 X C-(1	1)3(C))+(2	x ((H)₂(CO)	(C))+(1×CC	$(C)_2, \sigma = 18$	$C_p^{\circ} = S^{\circ} =$	216.90 305.31	214.93 312.53	1.97 -7.22	70AND/COU
	Literatus	e – Calculated	- Decidual	Reference	$\Delta_{f}S^{\circ} =$	303.31	- 607.86	- 1.22	70AND/COU
	Literatur	Calculated	- Residual	Reference	$\Delta_f G^\circ =$		- 140.76		
					$\ln K_{\rm f} =$		56.78		*
Gas phase $\Delta_i H^\circ =$	-257.95	-260.87	2.92	70HAR/HEA					
$C_p^{\circ} =$		124.27							
S° =	370.00	374.08	-4.08	65BUC/HER		e; Methyl ho			C ₈ H ₁₆ C
Δ _t S° -		410.00					\times C-(II) ₂ (CO)	(C) + $(1 \times CC)$)~(C)₂)+
$\Delta_{\mathbf{f}}G^{\circ} =$		- 138.63			(4×C-(1	$H)_2(C)_2), \sigma$	= 18		
$lnK_f =$		55.92				Literatu	re – Calculated	= Residual	Reference
Liquid phas	se								······································
$\Delta_t H^\circ =$	-296.51	-296.26	-0.25	70HAR/HEA	Gas phase				
$C_p^{\circ} =$	190.90	184.51	6.39	68AND/COU	$\Delta_t H^{\circ} =$		-321.55		
S° =	266.00	280.15	- 14.15	68AND/COU	$C_p^{\circ} =$		191.14		
$\Delta_f S^\circ =$		-503.93			S° =		491.14		
$\Delta_{\rm f}G^{\circ} =$		- 146.01			$\Delta_f S^\circ =$		-701.87		
$\ln K_{\rm f} =$		58.90			$\Delta_t G^\circ = $ $\ln K_t =$		-112.29 45.30		
	e; Methyl b	•	. (1 C. (TT)	C ₆ H ₁₂ O	Liquid phas	se			
	$-(C)_2$, $\sigma =$	\times C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂	(CO)(C))+	$\Delta_1 H^{\circ} =$	272.26	- 375.04	2.64	(COTTO
(1×00-	(C)2), 0° –	10			$C_p^{\circ} = S^{\circ} =$	273.26 373.84	276.90	-3.64	65OET
	Literatus	re – Calculated	= Residual	Reference	$\Delta_{f}S^{\circ} =$	3/3.04	369.80	4.04	65OET
	Literatu	Calculated	- Acsiduai	Reference	$\Delta_{\rm f}G^{\circ} =$		-823.21 -129.60		
					$\ln K_{\rm f} =$		52.28		
Gas phase							32.20		
$\Delta_f H^{\circ} =$	- 279.79	- 280.29	0.50	70HAR/HEA					
$C_p^o =$		145.36							
S° =		412.82			5-Nonanone	e; Di-n-buty	l ketone		C ₉ H ₁₈ O
$\Delta_f S^\circ =$		- 507.57			(2×C-(F	f(C) + (4	\times C-(H) ₂ (C) ₂)	$+(2\times C-(H)_2($	(CO)(C))+
$\Delta_{\mathbf{f}}G^{\circ} =$		- 128.96			(1×CO-	$(C)_2$, $\sigma =$	18	, ,,,,	. ,, ,,
lnK _f =		52.02			•	Literatur	re – Calculated	= Residual	Reference
Liquid pha	S A								
$\Delta_{\rm r} H^{\circ} =$	- 322.01	- 323.58	1.57	70HAR/HEA	Gas phase				
$C_p^{\circ} =$	213.38	216.06	-2.68	70AND/COU	$\Delta_t H^\circ =$	- 344.94	-343.39	- 1.55	70U A D /USE A
	308.11	305.04	3.07	70AND/COU	$C_p^{\circ} =$	J77.77	215.83	-1.55	70HAR/HEA
S° =	200.11	-615.35	5.07	10/11/D/COO	S° =		530.72		
S° = Δ ₆ S° =							JJU.12		
$\Delta_f S^{\circ} =$					م.ره =				
		-140.11 56.52			$\Delta_t S^\circ = \Delta_t G^\circ =$		- 798.60 - 105.29		

TABLE 18. Ketones (42) - Continued

TABLE 18. Ketones (42) - Continued

5-Nonanone; Di-n-butyl ketone (Continued)	C,H18O
$(2 \times C - (H)_3(C)) + (4 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(CO)(C)) +$	-
$(1 \times CO - (C)_2), \sigma = 18$	

Literatur	Literature — Calculated — Residual					
Liquid phase						
$\Delta_{\rm f}H^{\circ} = -398.24$	- 399.18	0.94	70HAR/HEA			
$C_{p}^{\circ} = 303.59$	306.19	-2.60	70AND/COU			
$S^{\circ} = 401.41$	409.67	-8.26	70AND/COU			
$\Delta_t S^{\circ} =$	-919.65					
$\Delta_{\rm f}G^{\circ} =$	- 124.99					
$lnK_t =$	50.42					

6-Undecanone; Di-n-pentyl ketone $C_{11}H_{22}O$ (2 × C-(H)₃(C)) + (6 × C-(H)₂(C)₂) + (2 × C-(H)₂(CO)(C)) + (1 × CO-(C)₂), $\sigma = 18$

Literatu	re – Calculated	Reference							
Gas phase									
$\Delta_i H^{\circ} = -387.41$	- 384.65	-2.76	70HAR/HEA						
$C_{p}^{\circ} =$	261.61								
S° =	609.04								
$\Delta_{\mathbf{f}}S^{\circ} =$	- 992.90								
$\Delta_{\rm f}G^{\circ} =$	-88.62								
$lnK_f =$	35.75								
Liquid phase									
$\Delta_{\rm f}H^{\circ} = -448.13$	- 450.64	2.51	70HAR/HEA						
$C_p^{\circ} =$	367.03		to the second se						
S° =	474.43								
$\Delta_t S^\circ =$	- 1127.51								
$\Delta_{\mathbf{f}}G^{\circ} =$	-114.47								
$lnK_f =$	46.18								

2-Tetradecanone; Methyl *n* -dodecyl ketone $(2 \times C - (H)_3(C)) + (1 \times CO - (C)_2) + (1 \times C - (H)_2(CO)(C)) + (10 \times C - (H)_2(C)_2), \sigma = 18$

	Literature - Calculated = Residua	l Reference
Gas phase		
$\Delta_t H^{\circ} =$	- 445.33	
$C_p^{\circ} =$	328.48	
S° =	726.10	
Δ _f S° =	- 1284.78	
$\Delta_i G^{\circ} =$	- 62.27	
$lnK_t =$	25.12	
: .		
Liquid phase		
$\Delta_t H^{\circ} =$	-529.42	
$C_p^o =$	459.42	
S° =	564.08	
$\Delta_t S^{\circ} =$	- 1446.80	
$\Delta_{\mathbf{f}}G^{\circ} =$	- 98.06	
$lnK_f =$	39.56	

2-Tetradecanone; Methyl *n*-dodecyl ketone (Continued) $(2 \times C-(H)_3(C)) + (1 \times CO-(C)_2) + (1 \times C-(H)_2(CO)(C)) + (10 \times C-(H)_2(C)_2), \ \sigma = 18$

	Literature - Calculated - Residual			Reference	
Solid phase $\Delta_t H^\circ = C_p^\circ =$	415.20	- 573.43 409.91	5.29	79SUN/SVE	

2-Pentadecanone; Methyl *n*-tridecyl ketone $(2 \times C - (H)_3(C)) + (1 \times CO - (C)_2) + (1 \times C - (H)_2(CO)(C)) + (11 \times C - (H)_2(C)_2), \sigma = 18$

	Literature – Calculated = R	ature - Calculated = Residual	
:			
Gas phase			
$\Delta_t H^{\circ} =$	-465.96		
$C_{p}^{\circ} =$	351.37		
S° =	765.26		
$\Delta_f S^\circ =$	- 1381.93		
$\Delta_t G^{\circ} =$	- 53.94		
$lnK_f =$	21.76		
Liquid phase $\Delta_{\ell}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = 0$	-555.15 489.84 596.46 -1550.73 -92.80 37.44		
$m_{K} =$	37.44		
Solid phase			· · · · · · · · · · · · · · · · · · ·
	- 602.84		

3-Methyl-2-butanone; Methyl isopropyl ketone $(3\times C-(H)_3(C))+(1\times C-(H)(CO)(C)_2)+(1\times CO-(C)_2)+\\(2\times -CH_3 \text{ corr (tertiary)})$

	Literatu	re – Calculated = Residual		Reference	
Gas phase Δ _t H° =	- 262.57	- 264.22	1.65	70HAR/HEA	
Liquid phas	e				
$\Delta_{\rm f}H^{\circ} =$	- 299.47	-303.84	4.37	70HAR/HEA	
$C_{p}^{\circ} =$		179.82			
S° ==		259.19			
$\Delta_{\rm f} S^{\circ} =$		- 524.89			
$\Delta_t G^\circ =$		-147.35			
$lnK_f =$		59.44			

C₆H₁₂O

C6H12O

C,H18O

TABLE 18. Ketones (42) - Continued

TABLE 18. Ketones (42) - Continued

2-Methyl-3-pentanone; Ethyl isopropyl ketone $(3 \times C-(H)_3(C)) + (1 \times C-(H)(CO)(C)_2) + (1 \times CO-(1 \times C-(H)_2(CO)(C)) + (2 \times -CH_3 \text{ corr (tertiary)})$	-(C) ₂)+
Literature – Calculated = Residual	Refe

Literature – Calculated = Residual			Reference	
Gas phase		200.00	0.04	700E I
$\Delta_{\rm f}H^{\circ} =$	-286.10	- 286.06	-0.04	70SEL
Liquid ph	asc			
$\Delta_t H^\circ =$	-325.90	- 327.98	2.08	70SEL
$C_p^{\circ} =$		209.11		
S° =		299.06		
$\Delta_f S^\circ =$		-621.33		
$\Delta_i G^{\circ} =$		-142.73		
$lnK_f =$		57.58		

3,3-Dimethyl-2-butanone; Methyl tert-butyl ketone $(4 \times C - (H)_3(C)) + (1 \times CO - (C)_2) + (1 \times C - (CO)(C)_3) +$ (3×-CH₃ corr (quaternary))

Literature - Calculated = Residual Reference Gas phase $\Delta_t H^\circ =$ -290.67-291.460.79 70HAR/HEA Liquid phase $\Delta_i H^{\circ} =$ -328.54-330.221.68 70HAR/HEA $C_{\rho}^{\circ} = S^{\circ} =$ 206.90 206.88 0.02 70AND/COU 70AND/COU 282.42 281.03 1.39 $\Delta_f S^\circ =$ -639.36 $\Delta_f G^\circ =$ - 139.60 $lnK_f =$ 56.31

2,2-Dimethyl-3-pentanone; Ethyl tert-butyl ketone C7H14O $(4 \times C-(H)_3(C)) + (1 \times C-(CO)(C)_3) + (1 \times CO-(C)_2) +$ $(1 \times C - (H)_2(CO)(C)) + (3 \times - CH_3 \text{ corr (quaternary)})$

Literature – Calculated = Residual			Reference	
Gas phase Δ _f H° =	-313.72	-313.30	-0.42	70SEL
Liquid pha	ıse			
$\Delta_{\rm f}H^{\circ} =$		-354.36	- 1.74	70SEL
C ^o _P −		236.17		
<i>S</i> ° =		320.90		
$\Delta_f S^\circ =$		- 735.80		
$\Delta_f G^\circ =$		134.98		
$lnK_c -$		54.45		

2,4-Dimethyl-3-pentanone; Diisopropyl ketone C7H14O $(4 \times C-(H)_3(C)) + (2 \times C-(H)(CO)(C)_2) + (1 \times CO-(C)_2) +$ (4×-CH₃ corr (tertiary))

	Literature – Calculated = Residual		Reference	
Gas phase	•			
$\Delta_t H^\circ =$	-311.10	-311.25	0.15	70SEL
Liquid ph	ase			
$\Delta_{\rm f} H^{\circ} =$	-352.92	- 359.70	6.78	70SEL
$C_p^{\circ} =$	233.70	233.71	-0.01	70AND/COU
S° =	318.00	317.97	0.03	70AND/COU
$\Delta_t S^\circ =$		- 738.73		
$\Delta_f G^\circ =$		- 139.45		
$lnK_f =$		56.25		

2,2,4-Trimethyl-3-pentanone; Isopropyl tert-

butyl ketone C₈H₁₆O $(5 \times C - (H)_{3}(C)) + (1 \times C - (CO)(C)_{3}) + (1 \times C - (H)(CO)(C)_{2}) +$

 $(1 \times CO - (C)_2) + (2 \times - CH_3 \text{ corr (tertiary)}) +$

(3×-CH₃ corr (quaternary))

	Literatu	ure – Calculated – Residual		Reference	
Gas phase Δ _t H° =	-338.30	- 338.49	0.19	70SEL	
Liquid pha	se				
$\Delta_t H^\circ =$	-381.60	-386.08	4.48	70SEL	
$C_{p}^{\circ} =$		260.77			
S° =		339.81			
$\Delta_f S^\circ =$		-853.20			
$\Delta_{\mathfrak{l}}G^{\circ} =$		-131.70			
$lnK_t =$					

2,2,4,4-Tetramethyl-3-pentanone; Di-tertbutyl ketone

•	
$(6 \times C-(H)_3(C)) + (2 \times C-(CO)(C)_3) + (1 \times CO-(C)_2) + (1 \times CO-(C)_3) + (1 \times C)_3 + (1 \times C$	+
(6×-CH ₃ corr (quat/quat))	

Literature – Calculated = Residual			Reference	
Gas phase Δ _i H° =		- 342.21	-3.60	70SEL
Liquid pha	ise			
$\Delta_{\rm f}H^{\circ} =$	-391.10	-389.96	-1.14	70SEL
$C_{P}^{\circ} =$		287.83		
s° -		361.65		
$\Delta_f S^\circ =$		- 967.67		
$\Delta_f G^{\circ} =$		-101.45		
$lnK_f =$		40.92		

TABLE 18. Ketones (42) — Conti	itinued
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TABLE 18. Ketones (42) - Continued

	() ₃ (C))+(2	ne × C-(H)(C)3) + + (1 × CO-(C)		C9H18O rr (tertiary))+		edione (Cor H)3(C))+(2	ntinued) 2 × CO-(C) ₂) + (1	1×C-(H)₂(C	C₅H₈O ₇ O) ₂)
(2×C-(H		e – Calculated :		Reference		Literatu	re – Calculated =	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 357.61	-356.77 215.89	-0.84	70SEL	Liquid pha $\Delta_t H^\circ = C_p^\circ =$	- 423.80	423.80 194.46	0.00	57NIC
$C_p^{\circ} = S^{\circ} =$	se 408.50	-409.74 300.23 398.97	1.24	70SEL		H) ₂ (C) ₂)+(opentanone	* *		
$\Delta_f S^\circ = \Delta_f G^\circ = 0$		- 930.35 - 132.36				Literatu	re – Calculated =	= Residual	Reference
ln <i>K</i> _f =		53.39			Gas phase $\Delta_t H^\circ =$	- 194.76	- 194.76	0.00	72WOL
	(C) + (2	eptanone × C-(C) ₄) + (6×) + (1 × CO-(C)		C ₁₁ H ₂₂ O quaternary)) +	Liquid pha Δ _t H° =		-237.40	0.00	72WOL
	Literatur	e – Calculated	= Residual	Reference					
Gas phase $\Delta_t H^\circ = C_p^\circ =$	-421.20	- 418.87 260.25	-2.33	71SEL			$2 \times C - (H)_2(CO)$ (rsc), $\sigma = 2$	(C))+(1×C0	C ₆ H ₁₀ O O-(C) ₂) +
						Literatu	re – Calculated =	Residual	Reference
Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	se 474.10	-477.06 350.91 416.05 -1185.89 -123.49 49.81	2.96	71SEL	Gas phase $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	- 227.74 109.66 322.17	- 227.74 109.66 322.17 - 467.65 - 88.31 35.62	0.00 0.00 0.00	72WOL 69STU/WES 69STU/WES
		one; Diacetyl × CO-(C)(CO))	C ₄ H ₆ O ₂	Liquid pha $ \Delta_t H^{\circ} = C_p^{\circ} = $		- 272.63 177.20	0.00 0.00	72WOL 80NAK/SUG
	Literatui	re – Calculated	= Residual	Reference	$S^{\circ} = \Delta_t S^{\circ} =$	221.98	221.98 - 567.84	0.00	80NAK/SUG
Gas phase $\Delta_f H^\circ =$	-327.10	- 327.10	0.00	54NIC/SZW	$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = $		-103.33 41.68		
Liquid phase $\Delta_t H^\circ =$		- 365.30	-0.00	54NIC/SZW			2 × C(H) ₂ (CO)(rsc)	(C)) + (1 × CC	C ₇ H ₁₂ O O-(C) ₂) +
2,4-Pentane	edione			C ₅ H ₈ O ₂		Literatur	re – Calculated =	Residual	Reference
(2×C-(H		\times CO–(C) ₂) + (re – Calculated :	,	O) ₂) Reference	Gas phase $\Delta_t H^\circ =$	- 248.11	- 248.11	0.00	72WOL
Gas phase Δ _t H° =	-380.60	380.60	0.00	70IRV/WAD	Liquid phase $\Delta_t H^\circ =$		- 297.65	0.00	72WOL

TABLE 18. Ketones (42) - Continued

TABLE 18. Ketones (42) - Continued

Cyclooctanone $(5 \times C-(H)_2(C)_2) + (2 \times C-(H)_2(CO)(C)) + (1 \times CO)(1 \times C)(CO)(C)$	C ₈ H ₁₄ O -(C) ₂) +	Cycloundecanone (Continued) $(8 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(CO)(C)) + (1 \times CO)(1 \times C)(CO)(C)$	C ₁₁ H ₂₀ O -(C) ₂)+
Literature - Calculated = Residual	Reference	Literature – Calculated = Residual	Reference
Gas phase $\Delta_t H^\circ = -272.17 -272.17$ 0.00	72WOL	Liquid phase $\Delta_t H^\circ = -386.35 -386.35 0.00$	72WOL
Liquid phase $\Delta_t H^\circ = -320.68 -320.68 0.00$	72WOL	Cyclododecanone $(9 \times C-(H)_2(C)_2) + (2 \times C-(H)_2(CO)(C)) + (1 \times CO)(1 \times Cyclododecanone)$	C ₁₂ H ₂₂ O -(C) ₂) +
Solid phase $\Delta_t H^{\circ} = -323.42 -323.42$ 0.00	72WOL	Literature – Calculated = Residual	Reference
Cyclononanone $(6 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(CO)(C)) + (1 \times CO)(C)$	C ₉ H ₁₆ O -(C) ₂)+	Gas phase $\Delta_t H^\circ = -349.11 -349.11$ 0.00	72WOL
(1 × cyclononanone) Literature − Calculated ≈ Residual	Reference	Liquid phase $\Delta_t H^\circ = -414.59 -414.59$ 0.00	72WOL
Gas phase $\Delta_{r}H^{\circ} = -279.70 -279.70 0.00$	72WOL	Solid phase $\Delta_t H^\circ = -431.33 -431.33 0.00$	72WOL
Liquid phase $\Delta_t H^{\circ} = -332.85 -332.85 0.00$	72WOL	Cyclopentadecanone $(1 \times CO - (C)_2) + (2 \times C - (H)_2(CO)(C)) + (12 \times C - (H)_2(CO)(C)(C)) + (12 \times C - (H)_2(CO)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)$	$C_{15}H_{28}O$ $(C)_2(C)_2) +$
Solid phase $\Delta_t H^\circ = -334.94 -334.93 -0.01$	72WOL	Literature – Calculated = Residual	Reference
Cyclodecanone $(7 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(CO)(C)) + (1 \times CO)(C)$	$C_{10}H_{18}O$ $-(C)_2) +$	Gas phase $\Delta_t H^\circ = -414.50 -414.50$ 0.00	38WOL/WEG
(1 × cyclodecanone) Literature – Calculated = Residual	Reference	Solid phase $\Delta_t H^\circ = -491.90 -491.90 0.00$	33RUZ/SCH
Gas phase $\Delta_t H^\circ = -305.06 -305.06$ 0.00	72WOL	Cycloheptadecanone $(1 \times CO-(C)_2) + (2 \times C-(H)_2(CO)(C)) + (14 \times C-(H)_2(CO)(C)(C)) + (14 \times C-(H)_2(CO)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)$	C ₁₇ H ₃₂ O
Liquid phase $\Delta_t H^\circ = -363.42 -363.42$ 0.00	72WOL	(1 × cycloheptadecanone rsc) Literature – Calculated = Residual	Reference
Cycloundecanone (8 × C-(H) ₂ (C) ₂) + (2 × C-(H) ₂ (CO)(C)) + (1 × CO) (1 × cycloundecanone)	$C_{11}H_{20}O$ $-(C)_2) +$	Gas phase $\Delta_t H^\circ = -460.30 -460.30$ 0.00	38WOL/WEG
Literature - Calculated = Residual	Reference	Solid phase $\Delta_t H^{\circ} = -536.00 - 536.00 = 0.00$	33RUZ/SCH
Gas phase $\Delta_t H^\circ = -322.00 -322.00 0.00$	72WOL		

	TABLE	18. Ketones (4	2) – Contin	ued
	$I)_3(C)) + (1$	phenyl ketone × CO-(C)(C _B))+(1×C _B -(C	C_8H_8O $O)(C_B)_2) +$
	Literatur	e – Calculated	= Residual	Reference
Gas phase Δ _t H° =		-106.53		
Liquid phas $\Delta_t H^\circ = C_p^\circ =$		- 141.53 227.62	- 0.97 - 0.02	61COL/LAT 39PHI
	CO)(C _B) ₂)	\times C-(H) ₂ (CO) + (5 \times C _B -(H)($^{\circ}$	C _B)₂)	P-(C)(C _B))+
	Literatui	e – Calculated	= Residual	Keterence
Gas phase Δ _t H° =		- 128.37		
Liquid phase $\Delta_t H^\circ = C_p^\circ =$		- 165.67 256.91	-1.53	61COL/LAT
	propanone;	Methyl benzyl	ketone	C ₃ H ₁₀ O
(1×C-(H	1)3(CO))+	$(1 \times CO - (C)_2) - (5 \times C_B - (H)(C_B)$	+ (1 × C-(H) ₂ (
	Literatur	re – Calculated	= Residual	Reference
Gas phase Δ _t H° =	-98.40	- 98.44	0.04	54NIC/SZW

Benzopheno (10×C _B -		yl ketone - (2×C _B -(CO)	$(C_B)_2$ + $(1 \times C_B)_2$	$C_{13}H_{16}$ CO-(C _B) ₂)
	Literatur	e – Calculated	= Residual	Reference
Gas phase Δ _t H° =	60.30	59.10	1.20	83DEK/VAN
Liquid phas $\Delta_t H^\circ =$		- 16.40	0.10	83DEK/VAN
Solid phase		24.40	0.00	
$\Delta_{\mathbf{f}}H^{\circ} = C_{p}^{\circ} =$	-34.40 224.81	- 34.40 224.85	0.00 -0.04	59COL/CAM 83DEK/VAN
(1×C-(H	$(C_B)_2 + (1)_3$; Phenyl p-toly × C _B -(H)(C _B) ₂ < C _B -(C)(C _B) ₂))+(2×C _B -(C	C ₁₄ H ₁₂ CO)(C _B) ₂) +
	Literatur	e – Calculated	= Residual	Reference
Gas phase Δ _t H° =		26.67		
Liquid phas Δ _ι H° =	е	-53.01		
Solid phase $\Delta_t H^\circ = C_p^\circ =$	77.80	- 73.77 248.91	-4.03	59COL/CAM
	$(C_B)_2 + (C_B)_2 + (1 > 1)$	(2×C _B -(CO)((C-(H) ₃ (C))+ e - Calculated	(1×C-(H)₂(C	
G1				
Gas phase $\Delta_t H^\circ =$		5.33		
Liquid phas Δ _t H° =	e -64.30	- 77.82	13.52	59COL/CAM
Δ _f Π =				
Solid phase $\Delta_t H^\circ =$		- 95.87		

TABLE 18. Ketones (42) - Continued

1-Phenyl-1-butanone; Propyl phenyl ketone

Liquid phase $\Delta_i H^\circ = -151.90$

Gas phase $\Delta_i H^{\circ} =$

Liquid phase $\Delta_{\mathbf{f}}H^{\circ} =$

 $C_p^{\circ} =$

-188.90

-152.08

 $(1 \times C - (H)_2(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) +$ $(1 \times CO - (C)(C_B)) + (1 \times C_B - (CO)(C_B)_2) + (5 \times C_B - (H)(C_B)_2)$ Literature - Calculated = Residual

-149.00

-191.40

287.33

0.18

2.50

54NIC/SZW

Reference

61COL/LAT

 $C_{10}H_{12}O$

TABLE 18. Ketones (42) - Continued

TABLE 19. Acids (89)

Diphenylethanedione; Benzil; Diphenyl diketone $(10 \times C_B-(H)(C_B)_2) + (2 \times C_B-(CO)(C_B)_2) + (2 \times C_B-(C_B)(C_B)_2) + (2 \times C_B-(C_B)(C_B)_2) + (2 \times C_B-(C_B)(C_B)(C_B)_2) + (2 \times C_B-(C_B)(C_B)(C_B)(C_B)_2) + (2 \times C_B-(C_B)(C_B)(C_B)(C_B)(C_B)_2 + (2 \times C_B)(C_B)(C_B)(C_B) + (2 \times C_B)(C_B)(C_B)(C_B)(C_B)(C_B)(C_B)(C_B)($	$C_{14}H_{10}O_2$ O-(CO)(C _B))		acid; Form H)(CO))+(ic acid (1×CO-(H)(O)), σ = 1	CH ₂ C
Literature - Calculated = Residual	Reference		Litera	ature-Calculate	ed = Résidual	Reference
Gas phase $\Delta_t H^{\circ} = -55.50 - 55.50 = 0.00$	59AIH	Gas phase $\Delta_r H^\circ = C_p^\circ = S^\circ =$	-378.70 45.23 248.74	-378.69 45.23 248.74	- 0.01 0.00 0.00	70KON/WAD 69STU/WES 69STU/WES
Solid phase $\Delta_t H^{\circ} = -153.90 - 153.90 0.00$	62PAR/MOS	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		- 92.61 - 351.08 141.62		
1,3-Diphenyl-1,3-propanedione; Dibenzoylmethane $(10 \times C_B-(H)(C_B)_2) + (2 \times C_B-(CO)(C_B)_2) + (2 \times C_B-(CO)(C_B)_2)$		Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = A_s G^\circ$	se -425.50 99.03 131.84	-428.06 102.92 132.96	2.56 -3.89 -1.12	64LEB 41STO/FIS 41STO/FIS
Literature - Calculated = Residual	Reference	$\Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$		-208.39 -365.93 147.61		
Gas phase $\Delta_t H^\circ = -159.26$			cid; Acetic : H) ₃ (C))+(1		+ (1 × O-(H)($C_{3}H_{4}O$ $CO)), \sigma = 3$
Liquid phase $\Delta_l H^\circ =$ -210.89 $C_p^\circ =$ 397.84		<u> </u>	Litera	ature-Calculate	ed = Residual	Reference
Solid phase $\Delta_i H^\circ = -224.90 -224.90 0.00$	65KOZ/SHI	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	-432.80 66.53 282.50	-433.80 66.52 282.49 -195.18	1.00 0.01 0.01	70KON/WAD 69STU/WES 69STU/WES
Cyclobutane-1,3-dione $(2 \times C-(H)_2(CO)_2) + (2 \times CO-(C)_2) + (1 \times \text{cyclobutane-1,3-dione rsc})$	C ₄ H ₄ O ₂	$\Delta_{f}G^{\circ} = \ln K_{f} =$		-375.61 151.52		
Literature – Calculated – Residual	Reference	Liquid pha $\Delta_l H^{\circ} = C_p^{\circ} =$	se -484.50 123.10	-482.62 119.28	-1.88 3.82	64LEB 82MAR/AND
Gas phase $\Delta_t H^\circ = -186.30 - 186.30 0.00$	78CHI/SHE	$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = -\infty$	158.00	154.30 -323.36 -386.21 155.79	3.70	82MAR/AND
Solid phase $\Delta_t H^{\circ} = -260.00 - 260.00 0.00$	78CHI/SHE				(C))+(1×CO-	C₃H₄O -(C)(O)) +
	•		Litera	ture-Calculate	d = Residual	Reference
		Gas phase $\Delta_t H^\circ = C_p^\circ =$	-455.70	-455.64 91.21	-0.06	70KON/WAD
		Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	58e - 508.50 152.80 191.00	-506.76 148.57 194.17 -419.81 -381.59 153.93	- 1.74 4.23 - 3.17	70KON/WAD 82MAR/AND 82MAR/AND

	Literature-Calculated	l = Residual	Reference		Litera	ature-Calculate	ed = Residual	Reference
Gas phase				Liquid pha	se			
$\Delta_t H^{\circ} =$	-468.76			$\Delta_t H^\circ = C_n^\circ =$	- 558.70 210.33	- 558.22 209.41	- 0.48 0.92	65ADR/DEK 65MCD/KIL
				$S^{\circ} =$	259.83	258.93	0.92	65MCD/KIL
Liquid phase				$\Delta_f S^\circ =$		-627.67		
$\Delta_i H^\circ =$	-552.87			$\Delta_{\mathfrak{l}}G^{\circ} =$		-371.08		
$C_p^{\circ} =$	171.36			$lnK_f =$		149.69		
S° =	151.48							
$\Delta_f S^\circ =$	-565.02							
$\Delta_{\rm f}G^{\circ} =$	-384.41			TT			G 17 G	
$lnK_f =$	155.07			(1×C-(1		× C-(H) ₂ (C) ₂)	C ₆ H ₁₂ O + (1 × C–(H) ₂ (
Solid phase				(1,700-	くくんひりょく	1×O-(H)(CO)	"	
	694.00 698.88	4.88	59SAV/GUN		Litera	ature-Calculate	ed = Residual	Reference
$C_p^{\circ} =$	127.83							
<i>s</i> ° =	147.30							
$\Delta_f S^\circ =$	-569.20			Gas phase				
	- 529.17			$\Delta_{\rm f}H^{\circ} =$	- 513.40	-517.53	4.13	79KRU/OON
-				~~				
	213.47	+ (1 × C-(H)-(C ₄ H ₆ O ₂	$C_{\rho}^{\circ} =$ Liquid pha $\Delta_{t}H^{\circ} =$ $C_{r}^{\circ} =$	se 585.60	159.88 - 583.95 239.83	-1.65	64LEB
Butanoic acid (1×C-(H) ₃ (1×CO-(C	213.47)		Liquid pha			-1.65	64LEB
Butanoic acid (1×C-(H) ₃ (1×CO-(C	213.47 ; Butyric scid (C)) + (1×C-(H) ₂ (C) ₂) + (1×O-(H)(CO)))	CO)(C))+	Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S_t G^\circ = S_$		- 583.95 239.83 291.31 - 731.60 - 365.82	-1.65	64LEB
$lnK_f =$ Butanoic acid $(1 \times C - (H)_3)$ $(1 \times CO - (C)_3)$ Gas phase	213.47 ; Butyric acid (C)) + (1 × C-(H) ₂ (C) ₂) + (O)) + (1 × O-(H)(CO)) Literature-Calculated) d = Residual	CO)(C)) + Reference	Liquid pha $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = $ Heptanoic $ (1 \times C - (1 + C_t)^2 + C_t)^2 = C_t C_t $	- 585.60 acid; Enant	- 583.95 239.83 291.31 - 731.60 - 365.82 147.57	C ₇ H ₁₄ O + (1 × C−(H) ₂ (2
Butanoic acid $(1 \times C - (H)_3)$ $(1 \times CO - (C)_3)$ Gas phase $\Delta_t H^{\circ} = C_p^{\circ} = C_p^{\circ} = C_p^{\circ}$ Liquid phasc	213.47 ; Butyric acid (C)) + (1 × C-(H) ₂ (C) ₂) + (O)) + (1 × O-(H)(CO)) Literature-Calculated 475.80 - 476.27 114.10) d = Residual 0.47	CO)(C))+ Reference 70KON/WAD	Liquid pha $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = $ Heptanoic $ (1 \times C - (1 + C_t)^2 + C_t)^2 = C_t C_t $	acid; Enant H) ₃ (C))+(4-(C)(O))+(- 583.95 239.83 291.31 - 731.60 - 365.82 147.57 thylic acid × C-(H) ₂ (C) ₂)	C ₇ H ₁₄ O + (1 × C-(H) ₂ (4	2 CO)(C))+
Butanoic acid $(1 \times C - (H)_3)$ $(1 \times CO - (C)_1 + (C)_2 + (C)_2 + (C)_3 + (C)_4 + (C)_4 + (C)_5 + (C)_6 + (C$	213.47 ; Butyric acid (C)) + (1 × C – (H) ₂ (C) ₂) + (O)) + (1 × O – (H)(CO)) Literature-Calculated 475.80 – 476.27 114.10) d = Residual	CO)(C)) + Reference	Liquid pha $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = $ Heptanoic $ (1 \times C - (1 + C_t)^2 + C_t)^2 = C_t C_t $	acid; Enant H) ₃ (C))+(4-(C)(O))+(- 583.95 239.83 291.31 - 731.60 - 365.82 147.57	C ₇ H ₁₄ O + (1 × C-(H) ₂ (4	2
Butanoic acid $(1 \times C - (H)_3)$ $(1 \times CO - (C)_1 + (C)_2 + (C)_3 + (C)_4 + (C)_4 + (C)_5 + (C)_6 + (C$	213.47 ; Butyric acid (C)) + (1 × C – (H) ₂ (C) ₂) + (O)) + (1 × O – (H)(CO)) Literature-Calculated 475.80 – 476.27 114.10 533.80 – 532.49 177.70 178.99 225.30 226.55	0.47	CO)(C)) + Reference 70KON/WAD 64LEB	Liquid pha $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = $ Heptanoic $ (1 \times C - (1 + C_t)^2 + C_t)^2 = C_t C_t $	acid; Enant H) ₃ (C))+(4-(C)(O))+(- 583.95 239.83 291.31 - 731.60 - 365.82 147.57 thylic acid × C-(H) ₂ (C) ₂)	C ₇ H ₁₄ O + (1 × C-(H) ₂ (4	2 CO)(C))+
Butanoic acid $(1 \times C - (H)_3)$ $(1 \times CO - (C)_3)$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phasc $\Delta_t H^\circ = C_p^\circ =$ $S^\circ = \Delta_t S^\circ =$	213.47 ; Butyric acid (C)) + (1 × C-(H) ₂ (C) ₂) + (O)) + (1 × O-(H)(CO)) Literature-Calculated 475.80 - 476.27 114.10 533.80 - 532.49 177.70 178.99 225.30 226.55 - 523.74	0.47 -1.31 -1.29	Reference 70KON/WAD 64LEB 82MAR/AND	Liquid pha $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1 \times C_t}{1 \times C_t}$ Heptanoic $(1 \times C_t)(1 \times C_t)$ Gas phase	acid; Enant H) ₃ (C))+(4-(C)(O))+(Litera	- 583.95 239.83 291.31 - 731.60 - 365.82 147.57 thylic acid × C-(H) ₂ (C) ₂) 1× O-(H)(CO)	$C_7H_{14}O$ $+ (1 \times C - (H)_2(0))$ $d = Residual$	2 CO)(C))+ Reference
Butanoic acid $(1 \times C - (H)_3)$ $(1 \times CO - (C)_1 \times CO - (C)_2 \times (C)_2 \times (C)_3 \times (C)_3$	213.47 ; Butyric acid (C)) + (1 × C-(H) ₂ (C) ₂) + (O)) + (1 × O-(H)(CO)) Literature-Calculated 475.80 - 476.27 114.10 533.80 - 532.49 177.70 178.99 225.30 226.55 - 523.74 - 376.34	0.47 -1.31 -1.29	Reference 70KON/WAD 64LEB 82MAR/AND	Liquid pha $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1 \times C_t}{1 \times C_t}$ Heptanoic $(1 \times C_t)(1 \times C_t)$ Gas phase $\Delta_t H^\circ = \frac{1 \times C_t}{1 \times C_t}$	acid; Enant H) ₃ (C))+(4-(C)(O))+(-583.95 239.83 291.31 -731.60 -365.82 147.57 thylic acid × C-(H) ₂ (C) ₂) 1× O-(H)(CO) ature-Calculate	C ₇ H ₁₄ O + (1 × C-(H) ₂ (4	2 CO)(C))+
Butanoic acid $(1 \times C - (H)_3)$ $(1 \times CO - (C)_1)$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phasc $\Delta_t H^\circ = C_p^\circ =$ $S^\circ = \Delta_t S^\circ =$	213.47 ; Butyric acid (C)) + (1 × C-(H) ₂ (C) ₂) + (O)) + (1 × O-(H)(CO)) Literature-Calculated 475.80 - 476.27 114.10 533.80 - 532.49 177.70 178.99 225.30 226.55 - 523.74	0.47 -1.31 -1.29	Reference 70KON/WAD 64LEB 82MAR/AND	Liquid pha $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1 \times C_t}{1 \times C_t}$ Heptanoic $(1 \times C_t)(1 \times C_t)$ Gas phase	acid; Enant H) ₃ (C))+(4-(C)(O))+(Litera	- 583.95 239.83 291.31 - 731.60 - 365.82 147.57 thylic acid × C-(H) ₂ (C) ₂) 1× O-(H)(CO)	$C_7H_{14}O$ $+ (1 \times C - (H)_2(0))$ $d = Residual$	CO)(C))+ Reference
Butanoic acid $(1 \times C - (H)_3)$ $(1 \times CO - (C)_1 \times CO - (C)_2 \times (C)_2 \times (C)_3 \times (C)_3$	213.47 ; Butyric acid (C)) + (1 × C-(H) ₂ (C) ₂) + (O)) + (1 × O-(H)(CO)) Literature-Calculated 475.80 - 476.27 114.10 533.80 - 532.49 177.70 178.99 225.30 226.55 - 523.74 - 376.34	0.47 -1.31 -1.29	Reference 70KON/WAD 64LEB 82MAR/AND	Liquid pha $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1 \times C_t}{1 \times C_t}$ Heptanoic $(1 \times C_t)(1 \times C_t)$ Gas phase $\Delta_t H^\circ = \frac{1 \times C_t}{1 \times C_t}$	acid; Enant H) ₃ (C)) + (4 -(C)(O)) + (Litera - 539.40	-583.95 239.83 291.31 -731.60 -365.82 147.57 thylic acid × C-(H) ₂ (C) ₂) 1× O-(H)(CO) ature-Calculate	$C_7H_{14}O$ $+ (1 \times C - (H)_2(0))$ $d = Residual$	CO)(C))+ Reference
Butanoic acid $(1 \times C - (H)_3)$ $(1 \times CO - (C)_1 \times CO - (C)_2 \times CO - (C)_3 \times CO - (C)_4 \times CO - (C)_5 \times CO - (C)_5 \times CO - (C)_5 \times CO - (C)_6 \times CO - $	213.47 ; Butyric acid (C)) + (1 × C-(H) ₂ (C) ₂) + (O)) + (1 × O-(H)(CO)) Literature-Calculated 475.80 - 476.27 114.10 533.80 - 532.49 177.70 178.99 225.30 226.55 - 523.74 - 376.34	0.47 -1.31 -1.29	Reference 70KON/WAD 64LEB 82MAR/AND	Liquid pha $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{12}$ Heptanoic $(1 \times C - (1 \times C) - (1 \times C) - (1 \times C)$ Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \frac{1}{12}$	acid; Enant H) ₃ (C)) + (4 -(C)(O)) + (Litera - 539.40	-583.95 239.83 291.31 -731.60 -365.82 147.57 thylic acid × C-(H) ₂ (C) ₂) 1× O-(H)(CO) ature-Calculate	$C_7H_{14}O$ $+ (1 \times C - (H)_2(0))$ $d = Residual$	2 CO)(C))+ Reference
Butanoic acid $(1 \times C - (H)_3)$ $(1 \times CO - (C)_1 \times CO - (C)_2 \times (C)_2 \times (C)_3 \times (C)_4 \times (C)_4$	213.47 ; Butyric acid (C)) + (1 × C-(H) ₂ (C) ₂) + (O)) + (1 × O-(H)(CO)) Literature-Calculated 475.80 - 476.27 114.10 533.80 - 532.49 177.70 178.99 225.30 226.55 - 523.74 - 376.34 151.81	0.47 -1.31 -1.29 -1.25	CO)(C)) + Reference 70KON/WAD 64LEB 82MAR/AND 82MAR/AND	Liquid pha $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Heptanoic $ (1 \times C - (1 \times C) - C) $ Gas phase $ \Delta_t H^\circ = C_p^\circ =$	acid; Enant H) ₃ (C)) + (4 -(C)(O)) + (Litera - 539.40	- 583.95 239.83 291.31 - 731.60 - 365.82 147.57 thylic acid × C-(H) ₂ (C) ₂) 1× O-(H)(CO) ature-Calculate	$C_7H_{14}O$ + $(1 \times C - (H)_2)(4$ = $(1 \times C - (H)_2)(4)$ = $(1 \times C - (H)_2)(4)$ = $(1 \times C - (H)_2)(4)$	2 CO)(C))+ Reference 79KRU/OON
In K_f = Butanoic acid $(1 \times C - (H)_3)$ $(1 \times CO - (C)_1$ Gas phase $\Delta_t H^\circ = C_p^\circ =$	213.47 ; Butyric acid (C)) + (1 × C-(H) ₂ (C) ₂) + (O)) + (1 × O-(H)(CO)) Literature-Calculated 475.80 - 476.27 114.10 533.80 - 532.49 177.70 178.99 225.30 226.55 - 523.74 - 376.34 151.81 d; Valeric acid	0.47 -1.31 -1.29 -1.25	CO)(C)) + Reference 70KON/WAD 64LEB 82MAR/AND 82MAR/AND	Liquid pha $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \ln K_t = \frac{1}{100}$ Heptanoic $(1 \times C - (1 \times C) - C_p^{\circ} = C_p^{\circ} = \frac{1}{100}$ Liquid pha $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \frac{1}{100}$	acid; Enant H) ₃ (C)) + (4 -(C)(O)) + (Litera - 539.40 se - 611.40	- 583.95 239.83 291.31 - 731.60 - 365.82 147.57 thylic acid × C-(H) ₂ (C) ₂) 1× O-(H)(CO) ature-Calculate - 538.16 182.77	$C_7H_{14}O$ + $(1 \times C - (H)_2)(4$ = $(1 \times C - (H)_2)(4)$ = $(1 \times C - (H)_2)(4)$	2 CO)(C))+ Reference 79KRU/OON 64LEB
In K_f = Butanoic acid $(1 \times C - (H)_3)$ $(1 \times CO - (C)_1$ Gas phase $\Delta_t H^\circ = C_p^\circ =$	213.47 ; Butyric acid (C)) + (1×C-(H) ₂ (C) ₂) + (O)) + (1×O-(H)(CO)) Literature-Calculated 475.80 - 476.27 114.10 533.80 - 532.49 177.70 178.99 225.30 226.55 - 523.74 - 376.34 151.81 d; Valeric acid a(C) + (2×C-(H) ₂ (C) ₂)-C(O) + (1×O-(H)(CO)	0.47 -1.31 -1.29 -1.25 +(1×C-(H) ₂ (CO)(C)) + Reference 70KON/WAD 64LEB 82MAR/AND 82MAR/AND	Liquid pha $\Delta_{t}H^{\circ} = C^{\circ}_{\rho} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{1}$ Heptanoic $(1 \times C - (1)(1 \times CO - C) + C)$ Gas phase $\Delta_{t}H^{\circ} = C^{\circ}_{\rho} = \frac{1}{1}$ Liquid pha $\Delta_{t}H^{\circ} = C^{\circ}_{\rho} = \frac{1}{1}$ $C^{\circ}_{\rho} = C^{\circ}_{\rho} = C^{\circ}_{\rho}$	acid; Enant H) ₃ (C)) + (4 -(C)(O)) + (Litera - 539.40 se - 611.40	- 583.95 239.83 291.31 - 731.60 - 365.82 147.57 thylic acid × C-(H) ₂ (C) ₂) 1× O-(H)(CO) ature-Calculate - 538.16 182.77 - 609.68 270.25 323.69 - 835.53	$C_7H_{14}O$ + $(1 \times C - (H)_2)(4$ = $(1 \times C - (H)_2)(4)$ = $(1 \times C - (H)_2)(4)$	2 CO)(C))+ Reference 79KRU/OON 64LEB
In K_f = Butanoic acid $(1 \times C - (H)_3)$ $(1 \times CO - (C)_1$ Gas phase $\Delta_t H^\circ = C_p^\circ =$	213.47 ; Butyric acid (C)) + (1×C-(H) ₂ (C) ₂) + (O)) + (1×O-(H)(CO)) Literature-Calculated 475.80 - 476.27 114.10 533.80 - 532.49 177.70 178.99 225.30 226.55 - 523.74 - 376.34 151.81 d; Valeric acid a(C) + (2×C-(H) ₂ (C) ₂)-	0.47 -1.31 -1.29 -1.25 +(1×C-(H) ₂ (CO)(C)) + Reference 70KON/WAD 64LEB 82MAR/AND 82MAR/AND	Liquid pha $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \ln K_t = \frac{1}{100}$ Heptanoic $(1 \times C - (1 \times C) - C_p^{\circ} = C_p^{\circ} = \frac{1}{100}$ Liquid pha $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \frac{1}{100}$	acid; Enant H) ₃ (C)) + (4 -(C)(O)) + (Litera - 539.40 se - 611.40	- 583.95 239.83 291.31 - 731.60 - 365.82 147.57 thylic acid × C-(H) ₂ (C) ₂) 1× O-(H)(CO) ature-Calculate - 538.16 182.77	$C_7H_{14}O$ + $(1 \times C - (H)_2)(4$ = $(1 \times C - (H)_2)(4)$ = $(1 \times C - (H)_2)(4)$	2 CO)(C))+ Reference 79KRU/OON 64LEB

TABLE 19. Acids (89) - Continued

TABLE 19. Acids (89) - Continued

 $\begin{array}{ll} \textbf{Octanoic acid; Caprylic acid} & C_8H_{16}O_2 \\ (1\times C-(H)_3(C)) + (5\times C-(H)_2(C)_2) + (1\times C-(H)_2(CO)(C)) + \\ (1\times CO-(C)(O)) + (1\times O-(H)(CO)) \end{array}$

	Literature-Calculated = Residual				
Gas phase $\Delta_t H^\circ = C_p^\circ =$		-558.79 205.66	4.89	79KRU/OON	
Liquid pha $\Delta_t H^\circ =$		- 635.41	-1.39	64LEB	
$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} = 0$	297.92	300.67 356.07 939.46	- 2.75	82SCH/MIL2	
$\Delta_f G^\circ = \ln K_f =$		-355.31 143.33			

Nonanoic acid; Pelargonic acid $\begin{array}{c} C_9H_{18}O_2\\ (1\times C-(H)_3(C))+(6\times C-(H)_2(C)_2)+(1\times C-(H)_2(CO)(C))+\\ (1\times CO-(C)(O))+(1\times O-(H)(CO)) \end{array}$

	Liter	ature-Calculate	Reference	
Gas phase $\Delta_t H^\circ =$	- 579.60	- 579.42	-0.18	68BAC/NOV
$C_p^{\circ} =$	•17.00	228.55		
Liquid pha				
Δ _I H° -	- 661.80	- 661.14	-0.66	64LEB
$C_{p}^{\circ} =$	326.37	331.09	-4.72	82SCH/MIL
S° =		388.45		
$\Delta_t S^\circ =$		- 1043.39		
$\Delta_r G^\circ =$		-350.05		
$lnK_t =$		141.21		

 $\begin{array}{ll} \textbf{Decanoic acid; Capric acid} & C_{10}H_{20}O_2\\ (1\times C-(H)_3(C)) + (7\times C-(H)_2(C)_2) + (1\times C-(H)_2(CO)(C)) + \\ (1\times CO-(C)(O)) + (1\times O-(H)(CO)) \end{array}$

	Liter	Reference		
Gas phase				
-	594.90	- 600.05	5.15	68BAC/NOV
$C_p^{\circ} =$		251.44		
Liquid ph $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = S^\circ =$	ase 684.30	-686.87 361.51 420.83 -1147.32 -344.80 139.09	2.57	65ADR/DEK

 $\begin{array}{ll} \textbf{Decanoic acid; Capric acid (Continued)} & C_{10}H_{20}O_2\\ (1\times C-(H)_3(C)) + (7\times C-(H)_2(C)_2) + (1\times C-(H)_2(CO)(C)) + \\ (1\times CO-(C)(O)) + (1\times O-(H)(CO)) \end{array}$

	Liter	ature-Calculated	Reference		
Solid phas					
$\Delta_{\rm f}H^{\circ} =$	-713.70	-716.26	2.56	65ADR/DEK	
$C_p^{\circ} =$		332.39			
S° =		296.40			
$\Delta_f S^\circ =$		- 1271.75			
$\Delta_{f}G^{\circ} =$		-337.09			
$lnK_f =$		135.98			

 $\begin{array}{ll} \mbox{Undecanoic acid; Undecylic acid} & C_{11} \mbox{H}_{22} \mbox{O}_2 \\ (1 \times C - (H)_3(C)) + (8 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) + \\ (1 \times CO - (C)(O)) + (1 \times O - (H)(CO)) \end{array}$

	Liter	Literature-Calculated = Residual					
Gas phase							
$\Delta_f H^\circ =$	- 614.60	-620.68	6.08	68BAC/NOV			
$C_p^{\circ} =$		274.33					
Liquid ph	ase						
	-710.20	- 712.60	2.40	65ADR/DEK			
$C_p^{\circ} =$		391.93					
S° =		453.21					
$\Delta_t S^\circ =$		- 1251.25					
$\Delta_{\mathbf{f}}G^{\circ} =$		-339.54					
$lnK_f =$		136.97					
Solid phas	se						
$\Delta_f H^\circ =$	- 735.90	- 745.67	9.77	65ADR/DEK			
C_p° -		354.31					
S° =		319.41					
$\Delta_f S^\circ =$		-1385.05					
$\Delta_t G^{\circ} =$		-332.72					
lnK_f -		134.22					

 $\begin{array}{c} \textbf{Dodecanoic acid; Lauric acid} & \textbf{C_{12}H}_{24}\textbf{O}_2\\ (1\times C-(H)_3(C)) + (9\times C-(H)_2(C)_2) + (1\times C-(H)_2(CO)(C)) +\\ (1\times CO-(C)(O)) + (1\times O-(H)(CO)) \end{array}$

	Literature-Calculated = Residual							
Gas phase								
$\Delta_l H^{} = -$ $C_p^{\circ} =$	642.00	641.31 297.22	- 0.69	68BAC/NOV				
Liquid phase								
$\Delta_t H^\circ = -$	737.90	- 738.33	0.43	65ADR/DEK				
$C_p^{\circ} =$		422.35						
s° =		485.59						
$\Delta_f S^* =$		- 1355.18						
$\Delta_f G^\circ =$		-334.28						
$lnK_f =$		134.85						

TABLE 19. Acids (89) - Continued

	auric acid (Contin (9 × C-(H) ₂ (C) ₂) + (1 × O-(H)(CO)	$+(1\times C-(H)_2(G))$	C ₁₂ H ₂₄ O ₂ CO)(C))+	(1×C-(H	$I)_3(C)) + (1$	iyristic acid (C 1×C-(H) ₂ (C) ₂ 1×O-(H)(CO)	$+(1\times C-(H)_2$	C ₁₄ H ₂₈ O ₂ (CO)(C))+
Lit	terature-Calculate	d = Residual	Reference		Liter	ature-Calculate	d = Residual	Reference
Solid phase				Solid phase				
$\Delta_t H^\circ = -774.60$ $C_p^\circ = 404.28$ $S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = -774.60$		0.48 28.05	65ADR/DEK 82SCH/MIL2	$\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$	-833.50 432.00	-833.90 420.07 388.44 -1724.96 -319.60 128.93	0.40 11.93	65ADR/DEK 82SCH/MIL2
	'ridecylic acid + (10×C-(H) ₂ (C) ₂ + (1×O-(H)(CO)		C ₁₃ H ₂₆ O ₂ (CO)(C))+	(1×C-(F	$I)_3(C)) + (1$	entadecylic acic 2×C-(H) ₂ (C) ₂ 1×O-(H)(CO)	$+(1\times C-(H)_2$	C ₁₅ H ₃₀ O ₂ (CO)(C))+
	terature-Calculate		Reference	`		ature-Calculate		Reference
Gas phase $\Delta_t H^\circ = -660.20$ $C_p^\circ =$	0 - 661.94 320.11	1.74	68BAC/NOV	Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 699.00	-703.20 365.89	4.20	68BAC/NOV
Liquid phase $ \Delta_t H^\circ = -763.50 $ $ C_p^\circ = \\ S^\circ = \\ \Delta_t S^\circ = \\ \Delta_t G^\circ = \\ \ln K_t = $	0 -764.06 452.77 517.97 -1459.12 -329.02 132.73	0.56	65ADR/DEK	Liquid phas $ \Delta_t H^\circ = C_p^\circ - S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se - 811.70	- 815.52 513.61 582.73 - 1666.98 - 318.51 128.48	3.82	65ADR/DEK
Solid phase $ \Delta_t H^{\circ} - 806.6 $ $ C_p^{\circ} = 387.6 $ $ S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = 806.6 $		- 2.11 - 10.54	65ADR/DEK 82SCH/MIL	Solid phase $\Delta_1 H^\circ = C_p^\circ = S^\circ = \Delta_1 S^\circ = \ln K_f = \ln K_f = $	861.70 443.29	- 863.31 441.99 411.45 - 1838.26 - 315.23 127.16	1.61 1.30	65ADR/DEK 82SCH/MIL
	; Myristic acid + (11 × C-(H) ₂ (C) ₂) + (1 × O-(H)(CO		C ₁₄ H ₂₈ O ₂ (CO)(C))+		I) ₃ (C)) + (1	almitic acid 3×C-(H) ₂ (C) ₂ 1×O-(H)(CO)		C ₁₆ H ₃₂ O ₂ (CO)(C))+
L	iterature-Calculate	d = Residual	Reference		Litera	ature-Calculate	d = Residual	Reference
Gas phase $\Delta_l H^\circ = -693.8$ $C_p^\circ =$	0 -682.57 343.00	-11.23	61DAV/MAL	Gas phase $\Delta_l H^\circ = C_p^\circ =$	737.00	-723.83 388.78	- 13.17	61DAV/MAL
Liquid phase $\Delta_t H^\circ = -788.8$ $C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	60 -789.79 483.19 550.35 -1563.05 -323.77 130.61	0.99	65ADR/DEK	Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se 838.10	- 841.25 544.03 615.11 - 1770.91 - 313.25 126.36	3.15	65ADR/DEK

TABLE 19. Acids (89) - Continued

Hexadecanoic acid; Palmitic acid (Continued)	$C_{16}H_{32}O_2$
$(1 \times C - (H)_3(C)) + (13 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO))$)(C))+
$(1 \times CO - (C)(O)) + (1 \times O - (H)(CO))$	

Literature-Calculated = Residual Reference Solid phase $\Delta_{\mathbf{f}}H^{\circ} =$ -891.50 -892.721.22 65ADR/DEK $C_p^{\circ} = S^{\circ} =$ -0.5582SCH/MIL2 463.91 463.36 434.46 $\Delta_f S^\circ =$ - 1951.56 $\Delta_{\rm f}G^{\,\circ} =$ -310.86

Octadecanoic acid; Stearic acid (Continued) C18H36O2 $(1 \times C - (H)_3(C)) + (15 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) +$ $(1 \times CO - (C)(O)) + (1 \times O - (H)(CO))$

	Liter	ature-Calculate	d = Residual	Reference
Solid phas	se			
$\Delta_{f}H^{\circ} =$	- 948.00	-951.54	3.54	65ADR/DEK
$C_p^{\circ} =$	501.55	507.75	-6.20	82SCH/MIL2
S° =		480.48		
$\Delta_f S^\circ =$		-2178.16		
$\Delta_f G^\circ =$		-302.12		
$lnK_f =$		121.87		

C₁₇H₃₄O₂ Heptadecanoic acid; Margaric acid

125.40

 $lnK_f =$

 $(1 \times C - (H)_3(C)) + (14 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) +$ $(1 \times CO - (C)(O)) + (1 \times O - (H)(CO))$

	Liter	ature-Calculate	ed = Residual	Reference
Gas phase				
$\Delta_{\mathbf{f}}H^{\circ} =$		- 744.46		
C _P =		411.67		
Liquid phase				
$\Delta_i H^\circ = -80$	65.60	- 866.98	1.38	65ADR/DEK
$C_p^{\circ} =$		574.45		
S° =		647.49		
$\Delta_{c}S^{\circ} =$		- 1874.84		
$\Delta_{\rm f}G^{\circ} =$		-308.00		
lnK _t -		124.24		
Solid phase				
$\Delta_1 H^{\circ} = -9$	24.40	- 922.13	-2.27	65ADR/DEK
$C_p^{\circ} = 4$	75.72	485.83	- 10.11	82SCH/MIL
S° =		457.47		
$\Delta_f S^\circ =$		- 2064.86		
$\Delta_t G^\circ -$		306.49		
$lnK_t =$		123.64		

Nonadecanoic acid; Nonadecylic acid

C19H38O2 $(1 \times C - (H)_3(C)) + (16 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) +$ $(1 \times CO-(C)(O)) + (1 \times O-(H)(CO))$

	Litera	ture-Calculate	d = Residual	Reference
Gas phase				
$\Delta_t H^\circ = -$	785.30	- 785.72	0.42	68BAC/NOV
C _p =		457.45		
Liquid phase				
$\Delta_t H^\circ = -1$	916.40	- 918.44	2.04	65ADR/DEK
$C_p^{\circ} =$		635.29		
S° =		712.25		
$\Delta_6 S^\circ =$		-2082.70		
$\Delta_f G^\circ =$		- 297.48		
$lnK_f =$		120.00		
Solid phase				
•	984.00	- 980.95	-3.05	65ADR/DEK
	525.34	529.67	-4.33	82SCH/MIL
S° =		503.49		
$\Delta_f S^\circ =$		-2291.46		
$\Delta_t G^{\circ} =$		- 297.75		
$lnK_f =$		120.11		

$C_{18}H_{36}O_2$ Octadecanoic acid; Stearic acid $(1 \times C - (H)_3(C)) + (15 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) + (1 \times CO - (C)(O)) + (1 \times O - (H)(CO))$

	Liter	ature-Calculate	ed = Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 781.20	-765.09 434.56	- 16.11	61DAV/MAL
Liquid ph	ase			
$\Delta_{f}H^{\circ} =$	-884.70	-892.71	8.01	65ADR/DEK
$C_p^{\circ} =$		604.87		
S° =		679.87		
$\Delta_f S^\circ =$		1978.77		
$\Delta_f G^\circ =$		-302.74		
$lnK_f =$		122.12		

Eicosanoic acid; Arachidic acid $C_{20}H_{40}O_2$ $(1 \times C - (H)_3(C)) + (17 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) +$ $(1 \times CO - (C)(O)) + (1 \times O - (H)(CO))$

	Litera	ture-Calculate	d = Residual	Reference
Gas phase $\Delta_t H^\circ = -8$	312.40	- 806.35	-6.05	61DAV/MAL
$C_p^{\circ} =$		480.34	3.52	
Liquid phase				
$\Delta_t H^\circ = -9$	940.00	- 944.17	4.17	65ADR/DEK
$C_p^{\circ} =$		665.71	,,,,,	00.12142211
S° =		744.63		
$\Delta_f S^\circ =$		- 2186.63		
$\Delta_r G^\circ =$		- 292.23		
$lnK_f =$		117.88		

TADIE	10	Acide	(80)	 Continued
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Eicosanoic acid; Arachidic acid (Continued) $(1 \times C - (H)_3(C)) + (17 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2)$	$C_{28}H_{49}O_2$ O)(C)) +	2,2-Dimethylpropanoic acid; Pivalic acid $C_5H_{10}O_2$ $(1 \times O - (H)(CO)) + (1 \times CO - (C)(O)) + (1 \times C - (CO)(C)_3) + (3 \times C - (H)_3(C)) + (3 \times - CH_3 \text{ corr (quaternary)})$
Literature-Calculated = Residual	Reference	Literature – Calculated = Residual Reference
Solid phase $\Delta_t H^\circ = -1011.90 -1010.36 -1.54$ $C_p^\circ = 545.14 551.59 -6.45$ $\Delta_t S^\circ = -2404.76$	65ADR/DEK 82SCH/MIL2	Gas phase $\Delta_t H^\circ = -491.30 -508.07$ 16.77 79KRU/OON
$\Delta_f G^\circ = -293.38$ $\ln K_f = 118.35$		Liquid phase $\Delta_t H^\circ = -564.50 - 564.86 = 0.36 = 54$ HAN/WAT $C_\rho^\circ = 200.23$ $S^\circ = 234.92$
2-Methylbutanoic acid (1 × O-(H)(CO)) + (1 × CO-(C)(O)) + (1 × C-(H)(C (2 × C-(H) ₃ (C)) + (1 × C-(H) ₂ (C) ₂) + (1 × -CH ₃ corr		$\Delta_{t}S^{\circ} = -651.68$ $\Delta_{t}G^{\circ} = -370.56$ $\ln K_{t} = 149.48$
Literature – Calculated = Residual	Reference	Solid phase $\Delta_t H^\circ = -565.00$ $C_p^\circ = 177.82$ 177.83 -0.01 $71KON/WAD$
Gas phase $\Delta_t H^\circ = -499.20$		
Liquid phase $ \Delta_t H^\circ = -554.50 -562.03 7.53 $ $ C_p^\circ = 203.59 $ $ S^\circ = 245.46 $ $ \Delta_t S^\circ = -641.14 $	54HAN/WAT	2-Propenoic acid; Acrylic acid $ (1\times O-(H)(CO)) + (1\times CO-(C_d)(O)) + (1\times C_d-(H)(CO)) + (1\times C_d-(H)_2), \ \sigma = 1 $ Literature – Calculated = Residual Reference
$\Delta_{t}G^{\circ} = -370.87$ $\ln K_{t} = 149.61$ 3-Methylbutanoic acid $(2 \times C - (H)_{3}(C)) + (1 \times C - (H)(C)_{3}) + (1 \times -CH_{3} \text{ corr } (1 \times C - (H)_{2}(CO)(C)) + (1 \times CO - (C)(O)) + (1 \times O - (E)(O)) + (E)(CO)(CO)(CO)(CO)(CO)(CO)(CO)(CO)(CO)(CO$		Gas phase $\Delta_t H^\circ = -332.41$ $C_\rho^\circ = 77.78 77.78 0.00 69STU/WES$ $S^\circ = 315.01 315.01 0.00 69STU/WES$ $\Delta_t S^\circ = -168.39$ $\Delta_t G^\circ = -282.20$ $\ln K_t = 113.84$
Literature – Calculated = Residual	Reference	Liquid phase
Gas phase $\Delta_t H^{\circ} = -504.10 -501.33 -2.77$ $C_p^{\circ} = 137.02$	79KRU/OON	$\Delta_t H^\circ = -383.88 -392.84 8.96$ 59SKI/SNE $C_p^\circ = 142.47$
Liquid phase $\Delta_t H^\circ = -561.60 - 561.32 - 0.28$ $C_t^\circ = 206.43$ $S^\circ = 253.58$	54HAN/WAT	Adamantane-1-carboxylic acid $C_{11}H_{16}O_2$ $(3 \times C - (H)(C)_3) + (6 \times C - (H)_2(C)_2) + (1 \times Adamantane rsc) +$ $(1 \times C - (CO)(C)_3) + (1 \times CO - (C)(O)) + (1 \times O - (H)(CO))$ Literature – Calculated = Residual Reference
$\Delta_t S^\circ = -633.02$ $\Delta_t G^\circ = -372.59$ $\ln K_t - 150.30$		Gas phase $\Delta_t H^\circ = -501.04$
		Solid phase $\Delta_i H^\circ = -643.08 -602.95 -40.13$ 73STE/CAR

Adamantane-2-carboxylic acid $(4 \times C-(H)(C)_3) + (5 \times C-(H)_2(C)_2) + (1 \times Adama: (1 \times C-(H)(CO)(C)_2) + (1 \times CO-(C)(O)) + (1 \times O-(C)(O)) + (1 \times O-(C)(O)(O)) + (1 \times O-(C)(O)(O)) + (1 \times O-(C)(O)(O)(O)) + (1 \times $	$C_{11}H_{16}O_2$ ntane rsc) + -(H)(CO)	Ethanedioic acid; Oxalic acid $(2 \times CO-(O)(CO)) + (2 \times O-(H)(CO))$	C₂H₂O
Literature – Calculated = Residual	Reference	Literature – Calculated = Residual	Reference
	<u> </u>	Gas phase	
Gas phase $\Delta_t H^\circ = -505.76$		$\Delta_t H^{\circ} = -732.00 -756.10$ 24.10	53BRA/COT
Solid phase $\Delta_t H^\circ = -627.18 -613.37 -13.81$	73STE/CAR	Liquid phase $\Delta_t H^{\circ} = -817.88$ $C_p^{\circ} = 156.90$	
(Z)-2-Butenedioic acid; Maleic acid $(2\times O-(H)(CO))+(2\times CO-(C_d)(O))+(2\times C_d-(C_d)(O))+(2\times C_d-(C_d)(C_d)(O))+(2\times C_d-(C_d)(C_d)(O))+(2\times C_d-(C_d)(C_d)(C_d)(C_d)+(2\times C_d-(C_d)(C_d)(C_d)+(2\times C_d)+(2\times C_d)+(2\times C$	C₄ H₄O₄ H)(CO))+	Solid phase $\Delta_t H^\circ = -829.70 -805.92 -23.78$	64WIL/SHI
Literature – Calculated = Residual	Reference	Propanedioic acid; Malonic acid $(2 \times O-(H)(CO)) + (2 \times CO-(C)(O)) + (1 \times C-(H)_2(O)) + $	C ₃ H ₄ O ₂
Gas phase $\Delta_t H^\circ = -679.40 -712.61$ 33.21	38WOL/WEG	Literature — Calculated = Residual	Reference
C _p ° = 104.77		Gas phase $\Delta_t H^\circ = -813.80$	
Liquid phase $\Delta_t H^\circ = -823.91$ $C_\rho^\circ = 228.20$		Liquid phase $\Delta_l H^o = -893.07$	
Solid phase $ \Delta_t H^\circ = -789.40 -811.13 21.73 $ $ C_p^\circ = 137.00 139.38 -2.38 $ $ S^\circ = 160.80 164.42 -3.62 $ $ \Delta_t S^\circ = -529.77 $ $ \Delta_t G^\circ = -653.18 $ $ \ln K_f = 263.49 $	38HUF/FOX 85WIL/CHA 85WIL/CHA	$C_r^{\circ} =$ 181.16 Solid phase $\Delta_t H^{\circ} = -891.00 -890.60 -0.40$ Butanedioic acid; Succinic acid	64WIL/SHI
		$(2 \times \Omega - (H)(CO)) + (2 \times CO - (C)(O)) + (2 \times C - (H)_2(O))$	(CO)(C))
(E)-2-Butenedioic acid; Fumaric acid $(2 \times O-(H)(CO)) + (2 \times CO-(C_d)(O)) + (2 \times C_d-(C_d)(O)) + (2 \times C_d-(C_d)(C_d)(O)) + (2 \times C_d-(C_d)(C_d)(O)) + (2 \times C_d-(C_d)(C_d)(O)) + (2 \times C_d-(C_d)(C_d)(O)) + (2 \times C_d-(C_d)(C_$	C ₄ H ₄ O ₄	Literature – Calculated = Residual	Reference
Literature – Calculated = Residual	Reference	Gas phase $\Delta_t H^\circ = -823.00 -826.76$ 3.76 $C_p^\circ = 130.96$	60DAV/THO
Gas phase $\Delta_t H^\circ = -675.80 -717.46$ 41.66 $C_p^\circ = 112.80$	38WOL/WEG	Liquid phase $\Delta_t H^\circ = -918.30$ $C_p^\circ = 224.18$	
Liquid phase $\Delta_t H^{\circ} = -829.18$ $C_p^{\circ} = 228.20$		$S^{\circ} = 221.74$ $\Delta_f S^{\circ} = -603.02$ $\Delta_f G^{\circ} = -738.51$ $\ln K_f = 297.91$	
Solid phase $ \Delta_t II^\circ = -812.20 -816.86 4.66 $ $ C_p^\circ = 142.00 139.38 2.62 $ $ S^\circ = 168.00 164.42 3.58 $ $ \Delta_t S^\circ = -529.77 $ $ \Delta_t G^\circ = -658.91 $ $ \ln K_t = 265.80 $	38HUF/FOX 85WIL/CHA 85WIL/CHA	Solid phase $ \Delta_t H^\circ = -940.40 \qquad 927.30 \qquad -13.10 $ $ C_p^\circ = 223.00 $ $ S^\circ = 157.28 $ $ \Delta_t S^\circ = -667.48 $ $ \Delta_t G^\circ = -728.29 $ $ \ln K_f = 293.79 $	72VAN/MAN

TABLE 19. Acids (89) - Continued

$(1 \times C - (H)$: acid; Glutaric)(CO))+(2×C0) ₂ (C) ₂))+(2×C-(H)	C ₅ H ₈ O ₄ ₂ (CO)(C))+	Heptanedioic acid; P $(2 \times O-(H)(CO)) +$ $(3 \times C-(H)_2(C)_2)$)+(2×C-(H	C ₇ H ₁₂ C) ₂ (CO)(C))+
	Literature – C	alculated:	= Residual	Reference	Literat	ure – Calculated	= Residual	Reference
Gas phase					Gas phase			
$\Delta_f H^{\circ} =$	-8	347.39			$\Delta_{\rm f} H^{\circ} =$	-888.65		
C _p =	1	153.85	·		C _p =	199.63		
Liquid phase	e				Liquid phase			
$\Delta_i H^\circ =$	-9	944.03			$\Delta_{\mathbf{f}}H^{\circ} =$	- 995.49		
$C_p^o =$	2	254.60			$C_p^{\circ} =$	315.44		
s° -	2	254.12			s° -	318.88		
$\Delta_f S^\circ =$	-7	706.95			$\Delta_f S^\circ =$	-914.81		
$\Delta_t G^{\circ} =$		733.25			$\Delta_{\mathbf{f}}G^{\circ} =$	-722.74		
$lnK_f =$		295.79			$lnK_f =$	291.55		
Solid phase				· · · · · · · · · · · · · · · · · · ·	Solid phase			
	-959.90 -9	956.71	-3.19	64WIL/SHI	$\Delta_t H^\circ = -1009.80$	- 1015.53	5.73	26VER/HAR
C_p° -		244.92	3.17	01111240111	$C_p^{\circ} =$	288.76	5.75	20 V LIQIDAN
S° =		180.29			S° =	226,31		
$\Delta_f S^\circ =$		780.78			$\Delta_{f}S^{\circ} =$	-1007.38		
$\Delta_f G^\circ =$		723.92			$\Delta_{\mathbf{f}}G^{\circ} =$	-715.18		
$\ln K_{\rm f} =$		723.92 292.02			$\ln K_{\rm f} =$	288.50		
		272.02				200.50		
mik _f =								
Hexanedioic	: acid; Adipic ac I)(CO)) + (2 × C I) ₂ (C) ₂) Literature – C	O-(C)(O)		$C_6H_{10}O_4$ $O_2(CO)(C)) +$ Reference	Octanedioic acid; Sul (2×O-(H)(CO))+ (4×C-(H) ₂ (C) ₂) Literate			$C_8H_{14}O$) ₂ (CO)(C)) + Reference
Hexanedioic (2×O-(H (2×C-(H	$(CO) + (2 \times C)_2$ $(C)_2$	O-(C)(O)) ₂ (CO)(C))+	(2×O-(H)(CO)) + (4×C-(H) ₂ (C) ₂) Literate	-(2×CO-(C)(O)) ₂ (CO)(C))+
Hexanedioic (2×O-(H (2×C-(H	I)(CO)) + (2 × C I) ₂ (C) ₂) Literature – C	O-(C)(O)) ₂ (CO)(C))+	(2×O-(H)(CO)) + (4×C-(H) ₂ (C) ₂) Literate Gas phase	-(2×CO-(C)(O)		Reference
Hexanedioic (2×O-(H (2×C-(H	$I)(CO)) + (2 \times C)$ $I)_2(C)_2)$ Literature – C -865.00	Calculated	= Residual	Reference	(2×O-(H)(CO)) + (4×C-(H) ₂ (C) ₂) Literate	- (2×CO-(C)(O) ure – Calculated =	= Residual) ₂ (CO)(C))+
Hexanedioic $(2 \times O - (H \times C - (H \times C + (H \times C) + (H \times C))))))))))))))))$	$I)(CO)) + (2 \times CI)_2(C)_2$ $Literature - CI$ $- 865.00$	CO-(C)(O) Calculated 868.02	= Residual	Reference	$(2 \times O-(H)(CO)) + (4 \times C-(H)_2(C)_2)$ Literate Gas phase $\Delta_t H^\circ = -894.90$	- (2×CO-(C)(O) ure – Calculated = - 909.28	= Residual	Reference
Hexanedioic $(2 \times O - (H \times C - (H \times C + (H \times C) + (H \times C)))))))))))))$	$I)(CO)) + (2 \times CI)_2(C)_2)$ $Literature - CI$ $- 865.00 - II$	CO-(C)(O) Calculated 868.02	= Residual	Reference	$(2 \times O-(H)(CO)) + (4 \times C-(H)_2(C)_2)$ Literate Gas phase $\Delta_t H^\circ = -894.90$ $C_\rho^\circ =$	- (2×CO-(C)(O) ure – Calculated = - 909.28	= Residual	Reference
Hexanedioic $(2 \times O - (H \times C - (H \times C + (H \times C) + (H \times C)))))))))))))$	$I)(CO)) + (2 \times C)$ $I)_2(C)_2)$ Literature – C $- 865.00 - 665.00$ Let $- 865.00 - 665.00$	CO-(C)(O) Calculated 868.02 176.74	= Residual	Reference	$(2 \times O - (H)(CO)) + (4 \times C - (H)_2(C)_2)$ Literate Gas phase $\Delta_l H^\circ = -894.90$ $C_p^\circ =$ Liquid phase $\Delta_l H^\circ =$	- (2×CO-(C)(O) ure - Calculated = - 909.28 222.52	= Residual	Reference
Hexanedioic $(2 \times O - (H \times C - (H \times C + (A \times C) + (A \times C)$	$I)(CO)) + (2 \times C)$ $I)_2(C)_2)$ Literature – C $- 865.00 - 665.00$ Let $- 865.00 - 665.00$	CO-(C)(O) Calculated 868.02 176.74 969.76 285.02	= Residual	Reference	$(2 \times O - (H)(CO)) + (4 \times C - (H)_2(C)_2)$ Literate Gas phase $\Delta_l H^\circ = -894.90$ $C^\circ_p = -894.90$ Liquid phase $\Delta_l H^\circ = -894.90$ $C^\circ_p = -894.90$ $C^\circ_p = -894.90$	- (2×CO-(C)(O) ure - Calculated = - 909.28 222.52 - 1021.22 345.86	= Residual	Reference
Hexanedioic $(2 \times O - (H \times C - (H \times C + (A \times C) + (A \times C)$	$I)(CO)) + (2 \times C)$ $I)_2(C)_2)$ Literature – C $- 865.00 - 6$ See	868.02 176.74 969.76 285.02 286.50	= Residual	Reference	$(2 \times O - (H)(CO)) + (4 \times C - (H)_2(C)_2)$ Literate Gas phase $\Delta_t H^\circ = -894.90$ $C^\circ_p = -894.90$ Liquid phase $\Delta_t H^\circ = -894.90$ $C^\circ_p = -894.90$	- (2×CO-(C)(O) ure - Calculated = - 909.28 222.52 - 1021.22 345.86 351.26	= Residual	Reference
Hexanedioic $(2 \times O - (H \times C - (H \times C - (H \times C + (H \times C) + (H \times C))))))))))))$	$I)(CO)) + (2 \times C)$ $I)_2(C)_2)$ Literature – C -865.00	868.02 176.74 969.76 285.02 286.50 810.88	= Residual	Reference	$(2 \times O - (H)(CO)) + (4 \times C - (H)_2(C)_2)$ Literate Gas phase $\Delta_t H^{\circ} = -894.90$ $C_p^{\circ} = -894.90$ Liquid phase $\Delta_t H^{\circ} = -894.90$	- (2×CO-(C)(O) ure - Calculated = - 909.28 222.52 - 1021.22 345.86	= Residual	Reference
Hexanedioic $(2 \times O - (H \times C - (H \times C + (A \times C) + (A \times C)$	$I)(CO)) + (2 \times C)$ $I)_2(C)_2)$ Literature - C $- 865.00 - 6$ See	868.02 176.74 969.76 285.02 286.50	= Residual	Reference	$(2 \times O - (H)(CO)) + (4 \times C - (H)_2(C)_2)$ Literate Gas phase $\Delta_t H^\circ = -894.90$ $C^\circ_p = -894.90$ Liquid phase $\Delta_t H^\circ = -894.90$ $C^\circ_p = -894.90$	- (2×CO-(C)(O) ure - Calculated = - 909.28 222.52 - 1021.22 345.86 351.26 - 1018.74	= Residual	Reference
Hexamedioic $(2 \times O - (H \times C - (H \times C - (H \times C + (H \times C) + (H \times C))))))))))))$	I)(CO)) + (2 × C I) ₂ (C) ₂) Literature – C – 865.00 –	20–(C)(O) Calculated 868.02 176.74 969.76 285.02 286.50 810.88 728.00	= Residual	Reference	$(2 \times O - (H)(CO)) + (4 \times C - (H)_2(C)_2)$ Literate Gas phase $\Delta_t H^\circ = -894.90$ $C^\circ_p = -894.90$ Liquid phase $\Delta_t H^\circ = -894.90$ $\Delta_t H^\circ = -894.90$ $\Delta_t H^\circ = -894.90$ $\Delta_t G^\circ = -894.90$ $\Delta_t G^\circ = -894.90$	- (2×CO-(C)(O) ure - Calculated = - 909.28 222.52 - 1021.22 345.86 351.26 - 1018.74 - 717.48	= Residual	Reference
Hexamedioic $(2 \times O - (H))$ $(2 \times C - (H))$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phas $\Delta_t H^\circ = C_p^\circ =$ $S^\circ = \Delta_t S^\circ =$ $\Delta_t G^\circ = \ln K_t =$ Solid phase	I)(CO)) + (2 × C I) ₂ (C) ₂) Literature – C – 865.00 –	CO-(C)(O) Calculated 868.02 176.74 969.76 285.02 286.50 810.88 728.00 293.67	= Residual	Reference 60DAV/THO	$(2 \times O - (H)(CO)) + (4 \times C - (H)_2(C)_2)$ Literate Gas phase $\Delta_l H^o = -894.90$ $C_p^o =$ Liquid phase $\Delta_l H^o = C_p^o = S^o = \Delta_l S^o = 1nK_l = S$ Solid phase	- (2×CO-(C)(O) ure - Calculated = - 909.28 222.52 - 1021.22 345.86 351.26 - 1018.74 - 717.48 289.43	= Residual	Reference 60DAV/THO
Hexamedioic $(2 \times O - (H))$ $(2 \times C - (H))$ Gas phase $\Delta_t H^{\circ} = C_p^{\circ} =$ Liquid phas $\Delta_t H^{\circ} = S_p^{\circ} =$ $\Delta_t S^{\circ} =$ $\Delta_t S^{\circ} =$ $\ln K_t =$ Solid phase $\Delta_t H^{\circ} =$	I)(CO)) + (2 × Cl) ₂ (C) ₂) Literature - Cl - 865.00 - Cl - 865.00 - Cl - 994.30 - Cl	20–(C)(O) Calculated 868.02 176.74 969.76 285.02 286.50 810.88 728.00 293.67	= Residual	Reference	$(2 \times O - (H)(CO)) + (4 \times C - (H)_2(C)_2)$ Literate Gas phase $\Delta_t H^\circ = -894.90$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ Solid phase $\Delta_t H^\circ = -1038.00$	- (2×CO-(C)(O) ure - Calculated = - 909.28 222.52 - 1021.22 345.86 351.26 - 1018.74 - 717.48 289.43 - 1044.94	= Residual	Reference
Hexamedioic $(2 \times O - (H))$ $(2 \times C - (H))$ Gas phase $\Delta_t H^{\circ} = C_p^{\circ} =$ Liquid phas $\Delta_t H^{\circ} = C_p^{\circ} =$ $\Delta_t S^{\circ} = \Delta_t S^{\circ} =$ $\ln K_t =$ Solid phase $\Delta_t H^{\circ} = C_p^{\circ} =$	I)(CO)) + (2 × Cl) ₂ (C) ₂) Literature - Cl - 865.00 - Cl - 865.00 - Cl - 994.30 - Cl	20–(C)(O) Calculated 868.02 176.74 969.76 285.02 286.50 810.88 728.00 293.67 986.12 266.84	= Residual	Reference 60DAV/THO	$(2 \times O-(H)(CO)) + (4 \times C-(H)_2(C)_2)$ Literate Gas phase $\Delta_t H^\circ = -894.90$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ Solid phase $\Delta_t H^\circ = -1038.00$ $C_p^\circ = G^\circ =$	- (2×CO-(C)(O) ure - Calculated = - 909.28 222.52 - 1021.22 345.86 351.26 - 1018.74 - 717.48 289.43 - 1044.94 310.68	= Residual	Reference 60DAV/THO
Hexanedioic $(2 \times O - (H))$ $(2 \times C - (H))$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = S_p^\circ = \Delta_t G^\circ =$ $\ln K_f =$ Solid phase $\Delta_t H^\circ = C_p^\circ = S_p^\circ =$ $S_p^\circ = S_p^\circ = S_p^\circ =$	I)(CO)) + (2 × Cl) ₂ (C) ₂) Literature – Cl – 865.00 –	20–(C)(O) Calculated 868.02 176.74 969.76 285.02 286.50 810.88 728.00 293.67 986.12 266.84 203.30	= Residual	Reference 60DAV/THO	$(2 \times O-(H)(CO)) + (4 \times C-(H)_2(C)_2)$ Literate Gas phase $\Delta_t H^\circ = -894.90$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t =$ Solid phase $\Delta_t H^\circ = -1038.00$ $C_p^\circ = S^\circ =$	- (2×CO-(C)(O) ure - Calculated = - 909.28 222.52 - 1021.22 345.86 351.26 - 1018.74 - 717.48 289.43 - 1044.94 310.68 249.32	= Residual	Reference 60DAV/THO
Hexamedioic $(2 \times O - (H))$ $(2 \times C - (H))$ Gas phase $\Delta_t H^{\circ} = C_p^{\circ} =$ Liquid phas $\Delta_t H^{\circ} = C_p^{\circ} =$ $\Delta_t S^{\circ} = \Delta_t S^{\circ} =$ $\ln K_t =$ Solid phase $\Delta_t H^{\circ} = C_p^{\circ} =$	I)(CO)) + (2 × Cl) ₂ (C) ₂) Literature – Cl – 865.00 –	20–(C)(O) Calculated 868.02 176.74 969.76 285.02 286.50 810.88 728.00 293.67 986.12 266.84	= Residual	Reference 60DAV/THO	$(2 \times O-(H)(CO)) + (4 \times C-(H)_2(C)_2)$ Literate Gas phase $\Delta_t H^\circ = -894.90$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ Solid phase $\Delta_t H^\circ = -1038.00$ $C_p^\circ = G^\circ =$	- (2×CO-(C)(O) ure - Calculated = - 909.28 222.52 - 1021.22 345.86 351.26 - 1018.74 - 717.48 289.43 - 1044.94 310.68	= Residual	Reference 60DAV/THO

Nonanedioic acid; Az (2 × O-(H)(CO)) + (5 × C-(H) ₂ (C) ₂))+(2×C-(H)	C ₉ H ₁₆ O ₄ O ₂ (CO)(C)) +	Undecanedioic acid $(2 \times O-(H)(CO)) + (7 \times C-(H)_2(C)_2)$	+(2×CO-(C)(O)))+(2×C-(H)	C ₁₁ H ₂₀ O ₂) ₂ (CO)(C)) +
Literati	ure – Calculated :	= Residual	Reference	Literat	ure – Calculated	= Residual	Reference
Gas phase				Gas phase			
$\Delta_t H^{\circ} =$	- 929.91			$\Delta_f H^\circ =$	-971.17		
$C_p^{\circ} =$	245.41			<i>C</i> _p ° =	291.19		
Liquid phase				Liquid phase			
$\Delta_t H^\circ =$	1046.95			$\Delta_{f}H^{\circ} =$	- 1098.41		
$C_p^{\circ} =$	376.28			$C_p^{\circ} =$	437.12		
S° =	383.64			S° =	448.40		
$\Delta_f S^\circ =$	-1122.67			$\Delta_{\rm f} S^{\circ} =$	- 1330.54		
$\Delta_{\rm f}G^{\circ} =$	-712.22			$\Delta_f G^\circ =$	-701.71		
$lnK_f =$	287.31			$lnK_f =$	283.07		
Solid phase				Solid phase			
$\Delta_f H^\circ = -1054.30$	1074.35	20.05	26VER/HAR	$\Delta_{\rm f} H^{\circ} = -1099.40$	- 1133.17	33.77	26VER/HAR
$C_p^{\circ} =$	332.60			$C_p^{\circ} =$	376.44		
S° =	272.33			S° =	318.35		•
$\Delta_f S^\circ =$	- 1233.98			$\Delta_f S^\circ =$	- 1460.59		
$\Delta_1 G^\circ =$	- 706.44			$\Delta_{\mathbf{f}}G^{\circ} =$	- 697.70		
$\ln K_{\ell} = \frac{1}{\ln K_{\ell}}$ Decanedioic acid; Se	284.97		C ₁₀ H ₁₈ O ₄	$lnK_f =$ Dodecanedioic acid	281.45		C ₁₂ H ₂₂ O ₄
$lnK_{\ell} = \frac{1}{2}$ Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$	284.97 bacic acid - (2×CO-(C)(O)) ₂ (CO)(C))+	Dodecanedioic acid (2×O-(H)(CO))+ (8×C-(H) ₂ (C) ₂)	+ (2×CO-(C)(O)) ₂ (CO)(C))+
$lnK_{\ell} = \frac{1}{2}$ Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$	284.97			Dodecanedioic acid (2×O-(H)(CO))+ (8×C-(H) ₂ (C) ₂)			C ₁₂ H ₂₂ O ₄) ₂ (CO)(C))+ Reference
$\begin{array}{c} \ln K_{\rm f} = \\ \\ \hline \\ \text{Decanedioic acid; Se} \\ (2 \times O - (H)(CO)) + \\ (6 \times C - (H)_2(C)_2) \\ \hline \\ \text{Literat} \\ \\ \hline \\ \text{Gas phase} \end{array}$	bacic acid - (2×CO-(C)(O)	= Residual	Reference	Dodecanedioic acid (2×O-(H)(CO))+ (8×C-(H) ₂ (C) ₂) Literat Gas phase	+ (2×CO-(C)(O) ure – Calculated	= Residual	Reference
$\begin{aligned} &\ln K_{\rm f} = \\ &\text{Decanedioic acid; Se} \\ &(2\times O-(H)(CO)) + \\ &(6\times C-(H)_2(C)_2) \end{aligned}$ Literat	284.97 bacic acid - (2×CO-(C)(O)) ₂ (CO)(C))+	Dodecanedioic acid (2×O-(H)(CO))+ (8×C-(H) ₂ (C) ₂) Literat	+ (2×CO-(C)(O)) ₂ (CO)(C))+
In K_1 = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_1 H^\circ = -921.90$	bacic acid -(2×CO-(C)(O) ure Calculated	= Residual	Reference	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^o = -976.90$	+ (2×CO–(C)(O) ure – Calculated – 991.80	= Residual	Reference
In K_1 = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_i H^{\circ} = -921.90$ $C_p^{\circ} =$	bacic acid -(2×CO-(C)(O) ure Calculated	= Residual	Reference	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -976.90$ $C_p^\circ =$	+ (2×CO–(C)(O) ure – Calculated – 991.80	= Residual	Reference
In K_f = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^{\circ} = -921.90$ $C_p^{\circ} =$ Liquid phase $\Delta_t H^{\circ} = -921.90$	284.97 bacic acid - (2 × CO–(C)(O) orre – Calculated - 950.54 268.30	= Residual	Reference	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -976.90$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = -976.90$	- (2×CO-(C)(O) ure - Calculated - 991.80 314.08	= Residual	Reference
In K_{ℓ} = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_{2}(C)_{2})$ Literat Gas phase $\Delta_{\ell}H^{\circ} = -921.90$ $C_{p}^{\circ} =$ Liquid phase	284.97 bacic acid - (2×CO-(C)(O) ure - Calculated - 950.54 268.30 - 1072.68	= Residual	Reference	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -976.90$ $C_p^\circ =$ Liquid phase	- (2×CO-(C)(O) ure - Calculated - 991.80 314.08	= Residual	Reference
In $K_{\rm f}$ = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^{\circ} = -921.90$ $C_p^{\circ} =$ Liquid phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} =$	284.97 bacic acid - (2×CO-(C)(O) ure - Calculated - 950.54 268.30 - 1072.68 406.70	= Residual	Reference	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -976.90$ $C^\circ_p =$ Liquid phase $\Delta_t H^\circ = C^\circ_p = S^\circ =$	- 991.80 314.08 - 1124.14 467.54 480.78	= Residual	Reference
In $K_{\rm f}$ = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^{\circ} = -921.90$ $C_p^{\circ} =$ Liquid phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} =$	284.97 bacic acid - (2×CO-(C)(O) oure - Calculated - 950.54 268.30 - 1072.68 406.70 416.02 - 1226.60	= Residual	Reference	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -976.90$ $C_\rho^\circ =$ Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ =$	- 991.80 314.08 - 1124.14 467.54 480.78 - 1434.47	= Residual	Reference
In $K_{\rm f}$ = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^{\circ} = -921.90$ $C_p^{\circ} =$ Liquid phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} =$	284.97 bacic acid - (2×CO-(C)(O) oure - Calculated - 950.54 268.30 - 1072.68 406.70 416.02	= Residual	Reference	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -976.90$ $C^\circ_p =$ Liquid phase $\Delta_t H^\circ = C^\circ_p = S^\circ =$	- 991.80 314.08 - 1124.14 467.54 480.78	= Residual	Reference
In $K_{\rm f}$ = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^{\circ} = -921.90$ $C_p^{\circ} =$ Liquid phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = inK_{\rm f} = 0$	284.97 bacic acid - (2 × CO-(C)(O) oure - Calculated - 950.54 268.30 - 1072.68 406.70 416.02 - 1226.60 - 706.97	= Residual	Reference	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -976.90$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = InK_t = InK_t$	- 991.80 314.08 - 1124.14 467.54 480.78 - 1434.47 - 696.45	= Residual	Reference
In K_f = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -921.90$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = 10K_f = 10K$	284.97 bacic acid -(2×CO-(C)(O) ure - Calculated -950.54 268.30 -1072.68 406.70 416.02 -1226.60 -706.97 285.19	= Residual 28.64	Reference 60DAV/THO	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -976.90$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t =$ Solid phase	- 991.80 314.08 - 1124.14 467.54 480.78 - 1434.47 - 696.45 280.94	= Residual	Reference 60DAV/THO
In K_f = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -921.90$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = 10K_f = 10K_f = 1000$ Solid phase $\Delta_t H^\circ = -1082.60$	284.97 bacic acid - (2×CO-(C)(O) oure - Calculated - 950.54 268.30 - 1072.68 406.70 416.02 - 1226.60 - 706.97 285.19 - 1103.76	= Residual	Reference	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -976.90$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ Solid phase $\Delta_t H^\circ = -1130.00$	- 991.80 314.08 - 1124.14 467.54 480.78 - 1434.47 - 696.45 280.94	= Residual	Reference
In K_f = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -921.90$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_f =$ Solid phase $\Delta_t H^\circ = -1082.60$ $C_p^\circ =$	284.97 bacic acid - (2×CO-(C)(O) oure - Calculated - 950.54 268.30 - 1072.68 406.70 416.02 - 1226.60 - 706.97 285.19 - 1103.76 354.52	= Residual 28.64	Reference 60DAV/THO	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -976.90$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t =$ Solid phase $\Delta_t H^\circ = -1130.00$ $C_p^\circ =$	- 991.80 314.08 - 1124.14 467.54 480.78 - 1434.47 - 696.45 280.94 - 1162.58 398.36	= Residual	Reference 60DAV/THO
In K_f = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -921.90$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_f =$ Solid phase $\Delta_t H^\circ = -1082.60$ $C_p^\circ = S^\circ = S^\circ$	284.97 bacic acid - (2×CO-(C)(O) oure - Calculated - 950.54 268.30 - 1072.68 406.70 416.02 - 1226.60 - 706.97 285.19 - 1103.76 354.52 295.34	= Residual 28.64	Reference 60DAV/THO	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -976.90$ $C_\rho^\circ = $ Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t = $ Solid phase $\Delta_t H^\circ = -1130.00$ $C_\rho^\circ = S^\circ = S^$	- 991.80 314.08 - 1124.14 467.54 480.78 - 1434.47 - 696.45 280.94 - 1162.58 398.36 341.36	= Residual	Reference 60DAV/THO
In $K_{\rm f}$ = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^{\circ} = -921.90$ $C_p^{\circ} =$ Liquid phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = 10K_{\rm f} = 1082.60$ $C_p^{\circ} = S^{\circ} = \Delta_t G^{\circ} = 1082.60$ $C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = 1082.60$ $C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = 1082.60$	284.97 bacic acid - (2×CO-(C)(O) oure - Calculated - 950.54 268.30 - 1072.68 406.70 416.02 - 1226.60 - 706.97 285.19 - 1103.76 354.52 295.34 - 1347.29	= Residual 28.64	Reference 60DAV/THO	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -976.90$ $C_\rho^\circ = $ Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = 10K_t = $ Solid phase $\Delta_t H^\circ = -1130.00$ $C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = 0$	- 991.80 314.08 - 1124.14 467.54 480.78 - 1434.47 - 696.45 280.94 - 1162.58 398.36 341.36 - 1573.89	= Residual	Reference 60DAV/THO
In $K_{\rm f}$ = Decanedioic acid; Se $(2 \times O - (H)(CO)) + (6 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^{\circ} = -921.90$ $C_p^{\circ} =$ Liquid phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t S^{\circ} = \ln K_{\rm f} =$ Solid phase $\Delta_t H^{\circ} = -1082.60$ $C_p^{\circ} = S^{\circ} = S$	284.97 bacic acid - (2×CO-(C)(O) oure - Calculated - 950.54 268.30 - 1072.68 406.70 416.02 - 1226.60 - 706.97 285.19 - 1103.76 354.52 295.34	= Residual 28.64	Reference 60DAV/THO	Dodecanedioic acid $(2 \times O - (H)(CO)) + (8 \times C - (H)_2(C)_2)$ Literat Gas phase $\Delta_t H^\circ = -976.90$ $C_\rho^\circ = $ Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t = $ Solid phase $\Delta_t H^\circ = -1130.00$ $C_\rho^\circ = S^\circ = S^$	- 991.80 314.08 - 1124.14 467.54 480.78 - 1434.47 - 696.45 280.94 - 1162.58 398.36 341.36	= Residual	Reference 60DAV/THO

TABLE 19. Acids (89) - Continued

Gas phase' $A_H^{+} = -1012.43$ $C_r^0 = 336.97$ Gas phase $A_H^{+} = -874.63$ Liquid phase $A_H^{+} = -1149.87$ $C_r^0 = 497.96$ $A_H^{+} = -972.01$ $C_r^0 = 275.84$ $A_S^0 = -1538.40$ $A_S^0 = -1538.40$ $A_S^0 = -834.89$ $A_G^0 = -723.90$ $A_G^0 = -720.90$ $A_$	Tridecanedioic acid $(2 \times O-(H)(CO)) +$ $(9 \times C-(H)_2(C)_2)$	(2×CO-(C)(O))+(2×C-(H _.	$C_{13}H_{24}O_4$ $O_2(CO)(C)) +$	2,2-Dime (2×O-(I	thylsuccinic H)(CO))+(2×CO-(C)(O))+(1×C-(H	C ₆ H ₁₀ O) ₂ (CO)(C))+
Gas phasés $\Delta H^+ = -1012.43$ $C_r^+ = 336.97$ Gas phase $\Delta H^+ = -1149.87$ $\Delta H^+ = -149.87$ ΔH	Literati	ire – Calculated :	= Residual	Reference) +	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Gas phasë					Literatu	re – Calculated	I = Residual	Reference
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		-1012.43							
Liquid phase $\Delta_H H^+ = -1149.87$ $\Delta_H H^- = -1149.87$ $\Delta_S H^- = -972.01$ $\Delta_S H^- =$	•						- 874 63		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	I iquid shaqo								
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		_11/0.97			Liquid abou				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$						SC	072.01		
					-				
Solid phase $A_tH^* = -1148.30 - 1191.99 $									
Solid phase $\Delta_t H^p = -1148.30 - 1191.99 - 43.69 - 26VER/HAR $	ma _f =	210.02							
$ \Delta H^{\circ} = -1148.30 - 1191.99 - 43.69 - 26VER/HAR \\ C_{f}^{\circ} - 304.28 \\ \Delta A^{\circ} = 364.37 \\ \Delta A^{\circ} = -1687.19 \\ \Delta A^{\circ} = -688.95 \\ \ln K_{f} = 277.92 $					InK _f =	 	291.69		
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		1191.99	43.69	26VER/HAR	Solid phase				
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	*		45.05	20 V EAVIE IN	•		- 977 56	- 10 24	33VFD/HAD
$\begin{array}{llllllllllllllllllllllllllllllllllll$						307.00		- 10.24	JJ V EN/IIAN
$\Delta_G^\circ = -688.95 \\ \ln K_t = 277.92$ $\begin{array}{rcl} \text{Methylbutanedioic acid; Methylsuccinic acid} & C_4H_6O_4 \\ (2\times O_{-}(H)(CO)) + (2\times CO_{-}(C)(O)) + (1\times C_{-}(H)_2(CO)(C)) + \\ (1\times C_{-}(H)(CO)) + (2\times CO_{-}(C)(O)) + (1\times C_{-}(H)_2(CO)(C)) + \\ (1\times C_{-}(H)(CO)(C)) + (1\times C_{-}(H)_2(C)) + \\ (1\times C_{-}(H)_2(C)) + (2\times C_{-}(H)_2(C)) + (2\times C_{-}(H)(CO)(C)_2) + \\ (2\times C_{-}(H)_2(C)) + (2\times C_{-}(H)(CO)) + (2\times C_{-}(H)(CO)(C)_2) + \\ (2\times C_{-}(H)_2(C)) + (2\times C_{-}(H)_2(C)) + (2\times C_{-}(H)(CO)(C)_2) + \\ (2\times C_{-}(H)_2(C)) + (2\times C_{-}(H)_2(C)) + (2\times C_{-}(H)(CO)(C)_2) + \\ (2\times C_{-}(H)_2(C)) + (2\times C_{-}(H)_2(C)) + (2\times C_{-}(H)(CO)(C)_2) + \\ (2\times C_{-}(H)_2(C)) + (2\times C_{-}(H)_2(C)) + (2\times C_{-}(H)(CO)(C)_2) + \\ (2\times C_{-}(H)_2(C)) + (2\times C_{-}(C)(C)) + (2\times C_{-}(H)(CO)(C)_2) + \\ (2\times C_{-}(H)_2(C)) + (2\times C_{-}(C)(C)(C)) + (2\times C_{-}(H)(CO)(C)_2) + \\ (2\times C_{-}(H)_2(C)) + (2\times C_{-}(H)_2(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)($					C _p		221.00		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$									
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$									
Gas phase $\Delta_t H^\circ = -849.69$ $\Delta_t H^\circ = -849.69$ Liquid phase $C_p^\circ = 273.38$ $S^\circ - 259.56$ $\Delta_t H^\circ = -947.84$ $\Delta_t S^\circ = -837.82$ $C_p^\circ = 248.78$ $S^\circ = 240.65$ $\Delta_t S^\circ = -727.58$ $\Delta_t S^\circ = -727.5$	$(1 \times C - (H)(CO)(C)$ $(1 \times -CH_3 \text{ corr (te)})$	$(1 \times C - (H)_3)$ (tiary))	(C))+			Literatui	e – Calculated	= Residual	Reference
$ \Delta_{t}H^{\circ} = -849.69 $ Liquid phase $ \Delta_{t}H^{\circ} = -977.38 $ $ C_{\rho}^{\circ} = 273.38 $ $ S^{\circ} = 259.56 $ $ \Delta_{t}H^{\circ} = -947.84 $ $ \Delta_{t}S^{\circ} = -837.82 $ $ \Delta_{t}G^{\circ} = -727.58 $ $ S^{\circ} = 240.65 $ $ \Delta_{t}S^{\circ} = -720.42 $ $ \Delta_{t}G^{\circ} = -733.05 $ $ \ln K_{t} = 295.71 $ Solid phase $ \Delta_{t}H^{\circ} = -977.50 -989.32 $	Literat	ure – Calculated	= Residual	Reference			- 872.62		
$ \Delta_{t}H^{\circ} = -849.69 $ Liquid phase $ \Delta_{t}H^{\circ} = -977.38 $ $ C_{\rho}^{\circ} = 273.38 $ $ S^{\circ} = 259.56 $ $ \Delta_{t}H^{\circ} = -947.84 $ $ \Delta_{t}S^{\circ} = -837.82 $ $ \Delta_{t}G^{\circ} = -727.58 $ $ S^{\circ} = 240.65 $ $ \Delta_{t}S^{\circ} = -720.42 $ $ \Delta_{t}G^{\circ} = -733.05 $ $ \ln K_{t} = 295.71 $ Solid phase $ \Delta_{t}H^{\circ} = -977.50 -989.32 $	Gas phase					· · · · · · · · · · · · · · · · · · ·			
Liquid phase $C_{p}^{h} = \begin{array}{ccccccccccccccccccccccccccccccccccc$		849.69			Liquid phas	se			
Liquid phase $S^{\circ} = 259.56$ $\Delta_t H^{\circ} = -947.84$ $\Delta_t G^{\circ} = -837.82$ $\Delta_t G^{\circ} = -727.58$ $\Delta_t G^{\circ} = -727.58$ $\Delta_t G^{\circ} = -720.42$ $\Delta_t G^{\circ} = -733.05$ $\Delta_t H^{\circ} = 295.71$ Solid phase $\Delta_t H^{\circ} = -958.20$ -958.31 0.11 33VER/HAR $C_p^{\circ} = 188.02$ Tacemic-2,3-Dimethyl-1,4-butanedioic acid; racemic-2,3-Dimethyl-1,4-butanedioic acid; racemic-2,3-Dimethyl-1,4-Dime					$\Delta_{\rm f}H^{\circ} =$		- 977.38		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$							273.38		
$C_{\rho}^{\circ} = 248.78 \\ S^{\circ} = 240.65 \\ \Delta_{h}S^{\circ} = -720.42 \\ \Delta_{f}G^{\circ} = -733.05 \\ \ln K_{f} = 295.71$ Solid phase $\Delta_{t}H^{\circ} = -958.20 - 958.31 \\ C_{\rho}^{\circ} = 188.02$ Solid phase $\Delta_{t}H^{\circ} = -958.20 - 958.31 \\ C_{\rho}^{\circ} = 188.02$ $C_{\rho}^{\circ} = 188.02$ $C_{\rho}^{\circ} = 160.11 33VER/HAR$ $C_{\rho}^{\circ} = 160.11 30VER/HAR$ $C_{\rho}^{\circ} = 160.11 30VER/HAR$ $C_{\rho}^{\circ} = 160.11 30VER/HAR$ $C_{\rho}^{\circ} = 160.11 30VER/HAR$ C_{ρ}°					S° =				
$S^{\circ} = 240.65 \\ \Delta_{t}S^{\circ} = -720.42 \\ \Delta_{t}G^{\circ} = -733.05 \\ \ln K_{t} = 295.71$ Solid phase $\Delta_{t}H^{\circ} = -958.20 - 958.31 \\ C^{\circ}_{p} = 188.02$ Solid phase $C^{\circ}_{p} = 188.02$ Solid phase $C^{\circ}_{p} = 188.02$ $C^{\circ}_{p} = 188.02$ $C^{\circ}_{p} = 188.02$ $C^{\circ}_{p} = 188.02$ racemic-2,3-Dimethyl-1,4-butanedioic acid; racemi	$\Delta_l H^{\circ} =$				$\Delta_{f}S^{\circ} =$				
$\Delta_t S^\circ = -720.42$ $\Delta_t G^\circ = -733.05$ $\ln K_t = 295.71$ Solid phase $\Delta_t H^\circ = -958.20 - 958.31 0.11 33\text{VER/HAR}$ $C_p^\circ = 188.02$ $racemic-2,3-Dimethyl-1,4-butanedioic acid; racemic-2,3-Dimethyl-1,4-butanedioic acid; racemic-2,3-D$									
$\Delta_{l}G^{\circ} = -733.05$ $\ln K_{l} = 295.71$ Solid phase $\Delta_{l}H^{\circ} = -977.50 - 989.32 11.82 33VER/K$ $C_{p}^{\circ} - 153.04$ Solid phase $C_{p}^{\circ} = 188.02$ $racemic-2,3-Dimethyl-1,4-butanedioic acid; racemic-2,3-Dimethyl-1,4-butanedioic $					$\ln K_{\rm f} =$		293.50		
Solid phase $\Delta_{t}H^{\circ} = -977.50 - 989.32 11.82 33VER/H$ Solid phase $\Delta_{t}H^{\circ} = -958.20 - 958.31 0.11 33VER/HAR$ $C_{p}^{\circ} = 188.02$ $racemic-2,3-Dimethyl-1,4-butanedioic acid; racemic-2,3-Dimethyl-1,4-butanedioic acid; race$									
Solid phase $\Delta_{t}H^{\circ} = -977.50 - 989.32 11.82 33\text{VER/H}$ $C_{p}^{\circ} = 188.02$ $\frac{\Delta_{t}H^{\circ} = -958.20 - 958.31}{C_{p}^{\circ} = 188.02} 0.11 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 33\text{VER/HAR}$ $\frac{\Delta_{t}H^{\circ} = -977.50 - 989.32}{C_{p}^{\circ} = 153.04} 11.82 11.8$									
Solid phase $\Delta_{t}H^{\circ} = -958.20 - 958.31 0.11 33\text{VER/HAR}$ $C_{p}^{\circ} = 188.02$ $racemic-2,3-Dimethyl-1,4-butanedioic acid; racemic-2,3-Dimethyl-1,4-butanedioic acid; racemic-2,3-Dimethyl-1,4-Dimethyl-1,4-Dimethyl-1,4-Dimethyl-1,4-Dimethyl-1,4-Dimethyl-1,4-Dimethyl-1,4-Dim$	$lnK_f =$	295.71							
Solid phase $\Delta_{t}H^{\circ} = -958.20 - 958.31 0.11 33\text{VER/HAR}$ $C_{p}^{\circ} = 188.02$ racemic-2,3-Dimethyl-1,4-butanedioic acid; racemic-2,3-Dimethylsuccinic acid $(2\times O-(H)(CO)) + (2\times CO-(C)(O)) + (2\times C-(H)(CO)(C)_{2}) + (2\times C-(H)_{3}(C)) + (2$					•	- 977.50		11.82	33VER/HAR
$C_{p}^{\circ} = 188.02$ racemic-2,3-Dimethyl-1,4-butanedioic acid; racemic-2,3-Dimethylsuccinic acid									
racemic-2,3-Dimethyl-1,4-butanedioic acid; racemic-2,3-Dimethylsuccinic acid $(2 \times O - (H)(CO)) + (2 \times C $	$\Delta_{\rm f} H^{\circ} = -958.20$		0.11	33VER/HAR					
2,3-Dimethylsuccinic acid $(2\times O-(H)(CO)) + (2\times CO-(C)(O)) + (2\times C-(H)(CO)(C)_2) + (2\times C-(H)_3(C)) + (2\times -CH_3 \text{ corr (tertiary)})$ $\text{Literature - Calculated = Residual} \qquad \text{Reference}$	$C_p^{\circ} =$	188.02							
$(2 \times O - (H)(CO)) + (2 \times CO - (C)(O)) + (2 \times C - (H)(CO)(C)_2) +$ $(2 \times C - (H)_3(C)) + (2 \times - CH_3 \text{ corr (tertiary)})$ $\text{Literature - Calculated = Residual} \qquad \text{Reference}$								acid; racemic	-
Literature – Calculated = Residual Reference					(2×O-(F	I)(CO))+(2×CO-(C)(O		$C_6H_{10}O_4$ $(CO)(C)_2) +$
					(2/10/(1)				Reference
Gas phase							- Calculated		1/010101100
$\Delta_i H^\circ = -872.62$									

2,3-Dimethy (2×O-(H)	vimethyl-1,4-butanedioic acylsuccinic acid (Continued (CO)) + (2 × CO-(C)(O)) - (CO) + (2 × -CH ₃ corr (ter	B) + (2 × C-(H)	$C_6H_{10}O_4$	Tetramethylbutanedic Tetramethylsuccini (2×O-(H)(CO)) + (4×C-(H) ₃ (C)) + (c acid (Continue (2×CO-(C)(O))+(2×C-(C	C ₈ H ₁₄ O. O)(C) ₃) +
	Literature - Calculated =	Residual	Reference	Literati	ure – Calculated	= Residual	Reference
				Solid phase $\Delta_t H^{\circ} = -1012.40$	1027.82	15.42	33VER/HAR
Liquid phase				$C_p^{\circ} =$	220.76	201.2	
$\Delta_t H^\circ =$	-977.38						
$C_p^{\circ} =$	273.38			***************************************			
S° =	259.56						
$\Delta_{\rm f} S^{\circ} =$	-837.82			Ethylbutanedioic acid	l; Ethylsuccinic	acid	C ₆ H ₁₀ O
$\Delta_{\mathbf{f}}G^{\circ} =$	-727.58			$(2\times O-(H)(CO))+$	$(2 \times CO - (C)(O)$	$(1 \times C - (H))$)(CO)(C) ₂)+
$lnK_f =$	293.50			$(1 \times C - (H)_2)(CO)(C$	$(1 \times C - (H)_2)$	$(C)_2$ + $(1 \times C$	-(H)₃(C))
Solid phase				Literat	ure – Calculated	= Residual	Reference
	983.80 - 989.32	5.52	33VER/HAR				
$C_r^{\circ} =$	153.04			Gas phase			
				$\Delta_t H^\circ =$	-868.06		
(2×O-(H) (1×C-(CC	anedioic acid; Trimethylsu (CO)) + (2×CO-(C)(O)) (O)(C) ₃) + (3×C-(H) ₃ (C)) + (corr (quaternary))	+ (1 × C-(H) + (1 × -CH ₃ c	corr (tertiary))+	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ =$	-971.39 279.20 273.03		
	Literature - Calculated =	Residual	Reference	$\Delta_t S^\circ =$	-824.35		
				$\Delta_{\mathbf{f}}G^{\circ} =$	-725.61		
				$\ln K_f =$	292.71		
Gas phase				muti —	272.11		
$\Delta_t H^\circ =$	- 897.56						
				Solid phase			
				$\Delta_t H^\circ = -989.20$	-985.38	-3.82	33VER/HAR
Liquid phase				$C_p^{\circ} =$	209.94	5.02	JJ V EJVIII IK
$\Delta_i H^\circ =$	- 1001.55						
$C_p^{\circ} =$	300.44						
S° =	281.40						
$\Delta_{\mathbf{f}}S^{\circ} =$	- 952.29			2,2-Diethyl-1,4-butan	edinic acid: 2.2-		
$\Delta_{\rm f}G^{\circ} =$	-717.62			Diethylsuccinic aci			C ₈ H ₁₄ O
$lnK_t =$	289.48			(2×O-(H)(CO))+	(2×CO-(C)(O)) ₂ (CO)(C))+
Solid phase				$(1 \times C - (CO)(C)_3) +$	-(2×C-(H)₂(C)₂	2)+(2×C-(H)) ₃ (C))
$\Delta_t H^\circ = -10$	000.80 - 1008.57	7.77	33VER/HAR	Literat	ure – Calculated	= Residual	Reference
$C_p^{\circ} =$	186.90	****	33 V EIGHT IIC				
				C1			
				Gas phase $\Delta_t H^\circ =$	-906.77		
Totus other!	tamadinia asida Tatuamat	hulomosimia	ou'd Cu o	·			
	butanedioic acid; Tetramet						
)(CO))+(2×CO-(C)(O))) ₃ (C))+(4×-CH ₃ corr (qu		J(~)3) 1	Liquid phase			
(+×C~(n)	/3(C)) ⊤ (¬ ∧ ¬Cn3 corr (qu	aternary))		$\Delta_t H^\circ \stackrel{\cdot}{=}$	- 1014.69		
	Literature - Calculated =	Residual	Reference	$C_p^{\circ} =$	336.68		
				S° =	327.25		
	•			$\Delta_{\rm f} S^{\circ} =$	- 1042.75		
Gas phase				$\Delta_{\rm f}G^{\circ} =$	- 703.79		
$\Delta_{\rm f}H^{\circ} =$	- 922.50			$lnK_f =$	283.91		
		·		Solid phase			
I ionid -b				Solid phase $\Delta_t H^\circ = -1032.70$	- 1027.68	-5.02	33VER/HAR
Liquid phase				<i>∆a1</i>	- 1027.00	- 3.02	JJ V L:R/MAX
$\Delta_{\rm f}H^{\circ} =$	-1025.72			-	265.72		
$\Delta_{i}H^{\circ} = C_{p}^{\circ} =$	- 1025.72 327.50			$C_p^{\circ} =$	265.72		
$\Delta_{\mathbf{f}}H^{\circ} = \\ C_{p}^{\circ} = \\ S^{\circ} = $	-1025.72 327.50 303.24			-	265.72	· · · · · · · · · · · · · · · · · · ·	
$\Delta_{i}H^{\circ} = C_{p}^{\circ} =$	- 1025.72 327.50			-	265.72		

TABLE 19. Acids (89) - Continued

meso-2,3-Diethylsu $(2 \times O-(H)(CO)) + (2 \times C-(H)_3(C)) + (3 \times C-(H)_3$	-(2×CO-(C)(O))	+ (2×C-(H)	C ₈ H ₁₄ O ₄)(CO)(C) ₂)+	Triethylbutanedioic a (2×O-(H)(CO)) + (1×C-(CO)(C) ₃) +	(2×CO-(C)(O) -(3×C-(H) ₂ (C)	$(1 \times C - (H))$ $(1 \times C - (H))$ $(2) + (3 \times C - (H))$)(CO)(C) ₂)+) ₃ (C))
Literat	ture Calculated =	Residual	Reference	Literate	ure – Calculated –––––	= Residual	Reference
				Liquid phase			
Gas phase				$\Delta_{\rm f}H^{\circ} =$	- 1067.78		
$\Delta_{\mathbf{f}}H^{\circ} =$	-909.36			$C_p^{\circ} =$	391.70		
				S° =	378.54		
				$\Delta_{\mathbf{f}}S^{\circ} =$	- 1264.08		
Liquid phase	1024.49			$\Delta_f G^\circ =$	- 690.89		
$\Delta_t H^{\circ} =$	- 1024.48			$lnK_f =$	278.70		
$C_p^{\circ} = S^{\circ} =$	334.22						
Δ ₁ S° =	324.32 1045.68			Calid mbass			
$\Delta_{f}G^{\circ} = $ $\Delta_{f}G^{\circ} = $				Solid phase $\Delta_t H^\circ = -1066.30$	1005 76	10.46	221/ED #14 D
$\ln K_{\rm f} =$	-712.71 287.50			$C_p^{\circ} =$	- 1085.76 252.66	19.46	33VER/HAR
Solid phase $\Delta_t H^\circ = -1019.20$ $C_p^\circ =$	1043.46 196.88	24.26	33VER/HAR	Tetraethylbutanedioid succinic acid (2×O-(H)(CO)) + (4×C-(H) ₂ (C) ₂) +	·(2×CO-(C)(O)))+(2×C-(C0	C ₁₂ H ₂₂ O ₄ O)(C) ₃) +
racemic-2,3-Diethyl-		id; racemic-	C ₈ H ₁₄ O ₄		ure - Calculated		Reference
2,3-Diethylsuccini (2×O-(H)(CO))		+ (2×C-(H					
$(2 \times O - (H)(CO))$ $(2 \times C - (H)_2(C)_2) +$	+(2×CO-(C)(O))			Gas phase $\Delta_t H^\circ =$	- 986.78		
(2×O-(H)(CO)) (2×C-(H) ₂ (C) ₂)+ Litera	+ (2×CO-(C)(O)) + (2×C-(H) ₃ (C)))(CO)(C) ₂)+	$\Delta_l H^{\circ} =$ Liquid phase			· · · · · · · · · · · · · · · · · · ·
(2×O-(H)(CO)) (2×C-(H) ₂ (C) ₂)+ Litera	+ (2 × CO-(C)(O)) + (2 × C-(H) ₃ (C)) ture – Calculated =)(CO)(C) ₂)+	$\Delta_t H^{\circ} =$ Liquid phase $\Delta_t H^{\circ} =$	-1111.08		
(2×O-(H)(CO)) (2×C-(H) ₂ (C) ₂)+ Litera	+ (2×CO-(C)(O)) + (2×C-(H) ₃ (C)))(CO)(C) ₂)+	$\Delta_t H^{\circ} =$ Liquid phase $\Delta_t H^{\circ} =$ $C_{\rho}^{\circ} =$	- 1111.08 449.18		· · · · · · · · · · · · · · · · · · ·
(2×O-(H)(CO)) (2×C-(H) ₂ (C) ₂)+ Litera	+ (2 × CO-(C)(O)) + (2 × C-(H) ₃ (C)) ture – Calculated =)(CO)(C) ₂)+	$\Delta_t H^{\circ} = {}$ Liquid phase $\Delta_t H^{\circ} = {} C_{\rho}^{\circ} = {} S^{\circ} = {}$	1111.08 449.18 432.76		· · · · · · · · · · · · · · · · · · ·
$(2 \times O - (H)(CO))$ $(2 \times C - (H)_2(C)_2) +$ Litera Gas phase $\Delta_t H^\circ =$	+ (2 × CO-(C)(O)) + (2 × C-(H) ₃ (C)) ture – Calculated =)(CO)(C) ₂)+	$\Delta_t H^{\circ} =$ Liquid phase $\Delta_t H^{\circ} =$ $C_{\rho}^{\circ} =$ $S^{\circ} =$ $\Delta_t S^{\circ} =$	1111.08 449.18 432.76 1482.49		· · · · · · · · · · · · · · · · · · ·
$(2 \times O - (H)(CO))$ $(2 \times C - (H)_2(C)_2) +$ Litera Gas phase $\Delta_t H^\circ =$ Liquid phase	+ (2×CO-(C)(O)) + (2×C-(H) ₃ (C)) ture – Calculated = - 909.36)(CO)(C) ₂)+	$\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	1111.08 449.18 432.76 1482.49 669.08		· · · · · · · · · · · · · · · · · · ·
$(2 \times O - (H)(CO))$ $(2 \times C - (H)_2(C)_2) +$ Litera Gas phase $\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$	+ (2×CO-(C)(O)) + (2×C-(H) ₃ (C)) ture - Calculated = - 909.36)(CO)(C) ₂)+	$\Delta_t H^{\circ} =$ Liquid phase $\Delta_t H^{\circ} =$ $C_{\rho}^{\circ} =$ $S^{\circ} =$ $\Delta_t S^{\circ} =$	1111.08 449.18 432.76 1482.49		· · · · · · · · · · · · · · · · · · ·
$(2 \times O - (H)(CO))$ $(2 \times C - (H)_2(C)_2) +$ Litera Gas phase $\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_\rho^\circ =$	+ (2 × CO-(C)(O)) + (2 × C-(H) ₃ (C)) ture - Calculated = - 909.36 - 1024.48 334.22)(CO)(C) ₂)+	$\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	1111.08 449.18 432.76 1482.49 669.08		
$(2 \times O - (H)(CO))$ $(2 \times C - (H)_2(C)_2) +$ Litera Gas phase $\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$	+ (2 × CO-(C)(O)) + (2 × C-(H) ₃ (C)) ture - Calculated = - 909.36 - 1024.48 334.22 324.32)(CO)(C) ₂)+	$\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	1111.08 449.18 432.76 1482.49 669.08		
$(2 \times O - (H)(CO))$ $(2 \times C - (H)_2(C)_2) + $ Litera Gas phase $\Delta_t H^\circ = $ Liquid phase $\Delta_t H^\circ = $ $C_t^\circ = $ $S^\circ = $ $\Delta_t S^\circ = $	+ (2 × CO-(C)(O)) + (2 × C-(H) ₃ (C)) ture - Calculated = - 909.36 - 1024.48 334.22 324.32 - 1045.68)(CO)(C) ₂)+	$\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Solid phase	1111.08 449.18 432.76 1482.49 669.08 269.90	21.54	22VED (IA D
$(2 \times O - (H)(CO))$ $(2 \times C - (H)_2(C)_2) +$ Litera Gas phase $\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$	+ (2 × CO-(C)(O)) + (2 × C-(H) ₃ (C)) ture - Calculated = - 909.36 - 1024.48 334.22 324.32)(CO)(C) ₂)+	$\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	1111.08 449.18 432.76 1482.49 669.08	31.56	33VER/HAR
$(2 \times O - (H)(CO))$ $(2 \times C - (H)_2(C)_2) + $ Litera Gas phase $\Delta_t H^\circ = $ Liquid phase $\Delta_t H^\circ = $ $C_\rho^\circ = $ $S^\circ = $ $\Delta_t S^\circ = $ $\Delta_t G^\circ = $ $\ln K_t = $ Solid phase	+ (2 × CO-(C)(O)) + (2 × C-(H) ₃ (C)) ture - Calculated = - 909.36 - 1024.48 334.22 324.32 - 1045.68 - 712.71 287.50	Residual	Reference	$\Delta_t H^{\circ} =$ Liquid phase $\Delta_t H^{\circ} =$ $C^{\circ}_{\rho} =$ $S^{\circ} =$ $\Delta_t S^{\circ} =$ $\Delta_t G^{\circ} =$ $\ln K_t =$ Solid phase $\Delta_t H^{\circ} = -1096.50$ $C^{\circ}_{\rho} =$	1111.08 449.18 432.76 1482.49 669.08 269.90	31.56	·
$(2 \times O - (H)(CO))$ $(2 \times C - (H)_2(C)_2) + $ Litera Gas phase $\Delta_t H^{\circ} = $ Liquid phase $\Delta_t H^{\circ} = $ $C_t^{\circ} = $ $S^{\circ} = $ $\Delta_t S^{\circ} = $ $\Delta_t G^{\circ} = $ $\ln K_t = $	+ (2 × CO-(C)(O)) + (2 × C-(H) ₃ (C)) ture - Calculated = - 909.36 - 1024.48 334.22 324.32 - 1045.68 - 712.71)(CO)(C) ₂)+	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = Solid phase$ $\Delta_t H^\circ = -1096.50$	- 1111.08 449.18 432.76 - 1482.49 - 669.08 269.90 - 1128.06 308.44		C₁H₄O₂
$(2 \times O - (H)(CO))$ $(2 \times C - (H)_2(C)_2) + $ Litera Gas phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Solid phase $\Delta_t H^\circ = -1026.30$	+ (2×CO-(C)(O)) + (2×C-(H) ₃ (C)) ture - Calculated = - 909.36 - 1024.48 334.22 324.32 - 1045.68 - 712.71 287.50 - 1043.46 196.88	Residual	Reference	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = Solid phase$ Solid phase $\Delta_t H^\circ = -1096.50$ $C_\rho^\circ = Solid phase$ Benzoic acid $(5 \times C_B - (H)(C_B)_2) - (1 \times O - (H)(CO))$	- 1111.08 449.18 432.76 - 1482.49 - 669.08 269.90 - 1128.06 308.44	C _B) ₂) + (1 × CC	C₁H₄O₂
$(2 \times O - (H)(CO))$ $(2 \times C - (H)_2(C)_2) + Litera$ Gas phase $\Delta_t H^\circ =$ $Liquid phase$ $\Delta_t H^\circ =$ $C_t^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Solid phase $\Delta_t H^\circ = -1026.30$ $C_t^\circ =$ $Triethylbutanedioic$ $(2 \times O - (H)(CO))$	+ (2×CO-(C)(O)) + (2×C-(H) ₃ (C)) ture - Calculated = - 909.36 - 1024.48 334.22 324.32 - 1045.68 - 712.71 287.50 - 1043.46 196.88	17.16 inic acid + (1 × C-(H	33VER/HAR C ₁₀ H ₁₈ O ₄)(CO)(C) ₂) +	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = Solid phase$ Solid phase $\Delta_t H^\circ = -1096.50$ $C_\rho^\circ = Solid phase$ Benzoic acid $(5 \times C_B - (H)(C_B)_2) - (1 \times O - (H)(CO))$	-1111.08 449.18 432.76 -1482.49 -669.08 269.90 -1128.06 308.44 +(1×C _B -(CO)(4)	C _B) ₂) + (1 × CC	C ₇ H ₆ O ₂ D-(O)(C _B)) +
$(2 \times O - (H)(CO))$ $(2 \times C - (H)_2(C)_2) + Litera$ Gas phase $\Delta_t H^\circ =$ $Liquid phase$ $\Delta_t H^\circ =$ $C_t^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Solid phase $\Delta_t H^\circ = -1026.30$ $C_t^\circ =$ $Triethylbutanedioic$ $(2 \times O - (H)(CO))$ $(1 \times C - (CO)(C)_3)$	+ (2×CO-(C)(O)) + (2×C-(H) ₃ (C)) ture - Calculated = - 909.36 - 1024.48 334.22 324.32 - 1045.68 - 712.71 287.50 - 1043.46 196.88 acid; Triethylsucci + (2×CO-(C)(O))	17.16 inic acid + (1 × C-(H) + (3 × C-(H)	33VER/HAR C ₁₀ H ₁₈ O ₄)(CO)(C) ₂) +	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = Solid phase$ Solid phase $\Delta_t H^\circ = -1096.50$ $C_\rho^\circ = S^\circ $	-1111.08 449.18 432.76 -1482.49 -669.08 269.90 -1128.06 308.44 +(1×C _B -(CO)(course-Calculated	C _B) ₂) + (1 × CC = Residual	C ₇ H ₆ O ₂ D-(O)(C _B))+ Reference

		······································							
Benzoic acid (5 × C _B -(1 (1 × O-(H	H)(C _B) ₂) + (H)(CO))	(1×C _B -(CO)(0			, ,	()(CO))+(1×CO-(O)(C₁ 1×C-(H)₃(C)		• • • • • • • • • • • • • • • • • • • •
	Literatur	e - Calculated	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Solid phase $\Delta_l H^\circ = C_p^\circ = S^\circ =$	-385.20 146.79 167.73	- 386.35 146.11 167.74	1.15 0.68 0.01	68CHU/ARM 76ARV/FAL 76ARV/FAL	Gas phase $\Delta_t H^\circ =$		- 327.18		
$\Delta_f S^\circ - \Delta_f G^\circ = \ln K_f =$		- 469.20 - 246.46 99.42			Liquid phase $\Delta_t H^\circ = C_p^\circ =$	e	-410.95 227.67		
	H)(CO)) + ((C)(C _B) ₂) + (corr)	$1 \times \text{CO-(O)}(\text{C}_{\text{E}}$ $(4 \times \text{C}_{\text{B}}(\text{H})(\text{C}_{\text{E}})$ $(4 \times \text{C}_{\text{B}}(\text{C})(\text{C}))$	₃) ₂) + (1 × C–(I		Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	- 429.20 169.03	- 425.72 170.17 196.18 - 577.07	-3.48 -1.14	61COL/BON 26AND/LYN
Gos phose	Literatui	re – Calculated	- Residual	Reference	$\Delta_t G^\circ = \ln K_t -$		-253.67 102.33		
Gas phase $\Delta_t H^\circ =$		-325.92							
Liquid phas $\Delta_t H^\circ = C_p^\circ =$	se	- 407.69 231.17			$(2 \times C_B - (0))$	(CO) + (CO) + (C) + (CO) + (I × CO-(O)(C ₁ 2 × C-(H) ₃ (C) (meta corr))+(3×C _B -(H	$((C_B)_2)$ +
Solid phase						Literatur	e – Calculated	= Residual	Reference
$\Delta_{i}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{i}S^{\circ} = \Delta_{i}S^{\circ$	-416.50 174.89	-420.72 170.17 196.18 -577.07	4.22 4.72	61COL/BON 26AND/LYN	Gas phase $\Delta_i H^\circ =$		-357.72		
$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = \\ -$		-248.67 100.31			Liquid phase $\Delta_l H^\circ = C_p^\circ =$	е	-441.04 258.57		
	$H)(CO)) + (C)(C_B)_2) +$	(1 × CO-(O)(C ₁ (1 × C-(H)₃(C)			-	- 450.40	-453.09	2.69	61COL/PER
	Literatu	re – Calculated	= Residual	Reference	$C_p^\circ = S^\circ = \Delta_p S^\circ = $		194.23 224.62 -684.94		
Gas phase $\Delta_t H^\circ =$		- 327.81			$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = \\ -$		-248.88 100.39		
Liquid phase $\Delta_c H^\circ - C_p^\circ =$	se	- 410.95 227.67			$(2 \times C_B - (C_B - (C_$	(CO) +	cid l×CO-(O)(C _l 2×C-(H) ₃ (C) meta corr)		
Solid phase Δ _f H° =	-426.10	- 423.72	-2.38	61COL/BON	***************************************	Literatur	c — Calculated	– Residual	Reference
$C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} =$	163.59	170.17 196.18 - 577.07 - 251.67	-6.58	26AND/LYN	Gas phase $\Delta_t H^\circ =$		-358.98		

TABLE 19. Acids (89) - Continued

	Literature - Calculated = Residual	Reference	Lit	erature – Calculated = Residual	Reference
Liquid phas			0 !!! !		
$\Delta_t H^\circ =$	-444.30		Solid phase	70 453.00 10.20	(1COL PED
$C_p^{\circ} =$	255.07		$\Delta_t H^\circ = -440$		61COL/PER
			$C_p^{\circ} =$	194.23	
_!:d _b			S° = Δ _t S° =	224.62 684.94	
Solid phase Δ _τ H° =	-458.50 -458.09 -0.41	61COL/PER	$\Delta_{f}G^{\circ} =$	- 084.94 - 248.88	
-	194.23	UICOLITER	$\ln K_{\rm f} =$	100.39	
$C_p^{\circ} = S^{\circ} -$	194.23 224.62		mx _t =	100.39	
$\Delta_{t}S^{\circ} =$	- 684.94				
$\Delta_{\rm f}G^{\circ} =$	-253.88				
$\ln K_{\rm f} =$	102.41		3,4-Dimethyl ben	zoic acid	C ₉ H ₁₀ C
•244.61	102.11			$(O) + (1 \times CO - (O)(C_B)) + (1 \times C_B - (O)(C_B)) + (O)(C_B) + (O)(C_B$	
				$(1 \times C_{B})$ + $(1 \times C_{B})$	
				(1) (1)	1)(CB)2) 1
2.5-Dimethy	yl benzoic acid	C ₉ H ₁₀ O ₂	(Tyronino con) i (i //meia coii)	
	$H(CO) + (1 \times CO - (O)(C_B)) + (1 \times C_B)$		Lie	erature - Calculated = Residual	Reference
	$C(C_B)_2 + (2 \times C - (H)_3(C)) + (3 \times C_B - $				
	$(1 \times meta \text{ corr})$	/(//			
(, . (2		Gas phase		
	Literature - Calculated = Residual	Reference	$\Delta_t H^\circ =$	- 358.98	
Gas phase			Liquid phase		
$\Delta_t H^\circ =$	- 358.98		$\Delta_t H^\circ =$	- 444.30	
			$C_p^{\circ} =$	255.07	
			·		
Liquid phas	se				
$\Delta_{f}H^{\circ} =$	-444.30		Solid phase		
$C_p^{\circ} =$	255.07		$\Delta_{\rm f}H^{\circ} = -468$		61COL/PER
			$C_p^{\circ} =$	194.23	
			S° =	224.62	
Solid phase			$\Delta_{t}S^{\circ} =$	- 684.94	
$\Delta_{\rm f}H^{\circ} =$	-456.10 -458.09 1.99	61COL/PER	$\Delta_t G^{\circ} =$	-253.88	
$C_p^{\circ} =$	194.23		$lnK_f =$	102.41	
S° =	224.62				
$\Delta_{\mathbf{f}}S^{\circ} =$	- 684.94				
$\Delta_f G^\circ =$	-253.88				
$lnK_f =$	102.41		3,5-Dimethyl ben		C,H ₁₀ C
				$(1 \times CO - (O)(C_B)) + (1 \times C_B - (O)(C_B)) + (O)(C_B - (O)(C_B)) + $	
				$(3)_2 + (2 \times C - (H)_3(C)) + (3 \times C_B - (H)_3(C))$	$(C_B)_2$ +
			(3×meta corr)		
•	yl benzoic acid	C ₉ H ₁₀ O ₂			D. C
	$H)(CO) + (1 \times CO - (O)(C_B)) + (1 \times C_B)$		Lit	erature – Calculated = Residual	Reference
	$(C)(C_B)_2 + (2 \times C - (H)_3(C)) + (3 \times C_B - (C))_3 + (2 \times C_B -$	11)(CB)2) T		**************************************	
(2 × onne	$p(corr) + (1 \times meta corr)$		Con ahoro		
	Litanatura Calaulata d. Davidual	Defenses	Gas phase	261.50	
	Literature - Calculated = Residual	Reference	$\Delta_t H^\circ =$	-361.50	
			• • • • •		
Gas phase			Liquid phase		
$\Delta_{\mathbf{f}}H^{\circ} =$	- 357.72		$\Delta_{\rm f}H^{\circ} =$	-447.56	
			$C_p^{\circ} =$	251.57	
Liquid pha	se.				
adaig bijg	5				
$\Delta_t H^{\circ} =$	- 441.04				

(1×O-(H	vi benzoic acid (Continued) i)(CO)) + $(1 \times CO - (O)(C_B)) + (1 \times C_B - (C)(C_B)_2) + (2 \times C - (H)_3(C)) + (3 \times C_B - (H)_3(C)) + (3 \times $			c acid (Continued) + $(1 \times CO-(O)(C_B)) + (1 \times CO-(H_3)(C)) + (3 \times C-(H_3)(C)) + (3 \times C-(H_3)(C))$		
	Literature - Calculated ≈ Residual	Reference	Litera	ture – Calculated = Res	sidual	Reference
Solid phase			Solid phase			
	-466.40 -459.09 -7.31	61COL/PER	$\Delta_{\rm f} H^{\circ} = -488.70$	-490.46	1.76	64COL/TUR
$C_p^{\circ} =$	194.23		$C_p^{\circ} =$	218.29		
S° =	224.62		s° =	253.06		
$\Delta_f S^{\circ} =$	- 684.94		$\Delta_{\mathbf{f}}S^{\circ} =$	- 792.81		
$\Delta_f G^\circ =$	-254.88		$\Delta_{\rm f}G^{\circ} =$	-254.08		
$\ln K_{\rm f} =$	102.82		$lnK_f =$	102.50		
$(1 \times O - (I \times O - ($	thyl benzoic acid H)(CO)) + $(1 \times CO - (O)(C_D)) + (1 \times C_D - (O)(C_D)) + (2 \times C_D - (O)($			$+(1 \times CO-(O)(C_B))+(1 \times C-(H)_3(C))+(2 \times C-(H)_3(C))$		
(3 × onno	corr) + (2× <i>meta</i> corr) Literature – Calculated = Residual	Reference	•	(2× <i>meta</i> corr) ture – Calculated = Res	sidual	Reference
Gas phase $\Delta_t H^\circ =$	- 389.52		Gas phase $\Delta_t H^\circ =$	- 389.52		
Liquid phas	se		Liquid phase			
$\Delta_t H^\circ =$	-474.39		$\Delta_{\mathbf{f}}H^{\circ} =$	-474.39		
$C_p^{\circ} =$	285.97		$C_p^{\circ} =$	285.97		
		me announce and execution are execution and execution and execution and execution and execution are execution are execution are execution are execution are execution are				
Solid phase		CACOL CITID	Solid phase	405 46	0.74	CLOOK TIVE
•		64COL/TUR	$\Delta_t H^\circ = -475.70$		9.76	64COL/TUR
$C_p^{\circ} =$	218.29		$C_p^{\circ} =$	218.29		
S° =	253.06		S° =	253.06		
$\Delta_{\mathbf{f}}S^{\circ} =$	-792.81		$\Delta_{\epsilon}S^{\circ} =$	- 792.81		
$\Delta_t G^\circ =$	- 249.08		$\Delta_{\mathbf{f}}G^{\circ} =$	-249.08		
$lnK_f =$	100.48		$lnK_f =$	100.48		
(1 × O-(I (3 × C _B -(thyl benzoic acid H)(CO)) + $(1 \times CO - (O)(C_B)) + (1 \times C_B - (C)(C_B)_2) + (3 \times C - (H)_3(C)) + (2 \times C_B - (H)_2(C)) + (2 \times meta\ corr)$		2,4,5-Trimethyl benz (1×O-(H)(CO))- (3×C _B -(C)(C _B) ₂) (2×ortho corr) + ($+(1 \times CO-(O)(C_B))+($ $+(3 \times C-(H)_3(C))+(2 \times C-(C_B))$	1×C _B −(CO) ×C _B −(H)(C	C ₁₀ H ₁₂ O ₂))+ _B) ₂)+
	Literature - Calculated = Residual	Reference	Litera	ture – Calculated = Res	idual	Reference
Gas phase			Gas phase			
$\Delta_{\rm f}H^{\circ} =$	-390.78		$\Delta_{\rm f}H^{\circ} =$	-390.78		
Liquid nhas	se		Liguid phase			
Liquid phas			Liquid phase	_ 177 65		
Liquid phas $\Delta_t H^\circ = C_p^\circ =$	- 477.65 282.47		Liquid phase $\Delta_t H^\circ = C_p^\circ =$	-477.65 282.47		

TABLE 19	Acids	(89) —	Continued
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2,4,5-Trimethyl benzoic acid (Continued) $ (1 \times O - (H)(CO)) + (1 \times CO - (O)(C_B)) + (1 \times C_{B'} - (O)(C_B)) + (1 \times C_{B'} - (O)(C_B)) + (2 \times C_{B'$		3,4,5-Trimethyl benzoic acid (Co $(1 \times O - (H)(CO)) + (1 \times CO - (CO)) + (1 \times CO - (CO)) + (1 \times CO - (CO)) + (1 \times CO) + ($	$(C_B) + (1 \times C_{B} - (1 \times C_{$	
Literature – Calculated = Residual	Reference	Literature – Calcul	ated = Residual	Reference
Solid phase		Solid phase		
$\Delta_t H^\circ = -495.70 -490.46 -5.24$	64COL/TUR	$\Delta_t H^\circ = -500.90 -492.40$	6 8.44	64COL/TUR
$C_p^{\circ} = 218.29$		$C_p^{\circ} = 218.29$		0.002,101.
$S^{\circ} = 253.06$		$S^{\circ} = 253.0$		
$\Delta_{b}S^{\circ} = -792.81$		$\Delta_t S^\circ = -792.8$		
· ·		=		
$\Delta_{\rm f}G^{\circ} = -254.08$		-		
$\ln K_{\rm f} = 102.50$		$\ln K_t = 103.36$	J	
2,4,6-Trimethyl benzoic acid $(1 \times O-(H)(CO)) + (1 \times CO-(O)(C_B)) + (1 \times C_B + (3 \times C_B-(C)(C_B)_2) + (3 \times C-(H)_3(C)) + (2 \times C_B-(2 \times ortho\ corr) + (3 \times meta\ corr)$		2,3,4,5-Tetramethyl benzoic acid $(1 \times O - (H)(CO)) + (1 \times CO - (CO)(CO) + (1 \times CO) + (1 \times CO)(CO) + (1 \times CO)(CO)(CO) + (1 \times CO)(CO)(CO) + (1 \times CO)(CO)(CO) + (1 \times CO)(CO)(CO) + (1 \times CO)(CO)(CO)(CO) + (1 \times CO)(CO)(CO)(CO) + (1 \times CO)(CO)(CO)(CO)(CO)(CO)(CO)(CO)(CO)(CO)($	$_3(C)) + (1 \times C_B - (H))$	
Literature - Calculated = Residual	Reference	Literature – Calcul	ated = Residual	Reference
Gas phase				
$\Delta_t H^{\circ} = -391.41$		Gas phase $\Delta_t H^\circ = -421.93$	5	
Liquid phase				
$\Delta_t H^{\circ} = -477.65$		Liquid phase		
$C_p^o = 282.47$		$\Delta_t H^\circ = -507.74$	1	
Cp - 202.47		$C_p^{\circ} = 313.33$		
Solid phase				
$\Delta_i H^{\circ} = -477.90 -488.46 $ 10.56	64COL/TUR	Solid phase		
$C_p^{\circ} = 218.29$		$\Delta_t H^\circ = -514.40 -515.83$	3 1.43	64COL/PER
S° = 253.06		$C_p^{\circ} = 242.33$		0.002,121
$\Delta_{\rm f}S^{\circ} = -792.81$		$S^{\circ} = 281.50$		
$\ln K_{\rm f} = 101.69$		$\Delta_f G^\circ = -247.29$ $\ln K_f = 99.76$		
3,4,5-Trimethyl benzoic acid $(1 \times O - (H)(CO)) + (1 \times CO - (O)(C_B)) + (1 \times C_B - (O)(C_B$	(H)(C _B) ₂)+	2,3,4,6-Tetramethyl benzoic acid $(1 \times O - (H)(CO)) + (1 \times CO - (C)(C \times C) + (4 \times C - (H)(C \times C)) + (4 \times C - (H)(C \times C)) + (4 \times C)$	$_3(C)) + (1 \times C_B - (H$	C ₁₁ H ₁₄ O CO)) + t)(C _B) ₂) +
Literature – Calculated = Residual	Reference	Literature – Calcula	ated = Residual	Reference
Gas phase				
$\Delta_i H^{\circ} = -390.15$		Gas phase $\Delta_t H^\circ = -421.99$	5	
Liquid phase				
Liquid phase $\Delta H^{\circ} = -477.65$		Liquid phase		
Liquid phase $\Delta_t H^{\circ} = -477.65$ $C_{\rho}^{\circ} = 282.47$		Liquid phase $\Delta_t H^\circ = -507.74$	1	

$(1 \times O - (H))(CC)$ $(4 \times C_B - (C))(C)$	hyl benzoic acid (Con O)) + $(1 \times CO - (O)(C_B + (O)) + (4 \times C - (H)_3(C)) + (4 \times Meta \ COT)$	$(1) + (1 \times C_B - (1))$			I)(CO))+(C)(C _B) ₂)+	cid (1×CO-(O)(C ₁ (5×C-(H) ₃ (C)		
,Li	terature – Calculated	= Residual	Reference		Literatur	re – Calculated	= Residual	Reference
Solid phase $\Delta_t H^\circ = -50^\circ$ $C_p^\circ =$	7.70 -515.83 242.35	8.13	64COL/PER	Gas phase $\Delta_t H^\circ =$		- 452.49		***************************************
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t =$	281.50 900.68 247.29 99.76			Liquid phas $\Delta_t H^\circ = C_p^\circ =$	se 	- 537.83 344.27		
$(1 \times O - (H)(C) + (4 \times C_B - (C)(C))$	thyl benzoic acid O)) + $(1 \times CO - (O)(C_E)$ $(C_B)_2$) + $(4 \times C - (H)_3(C))$ r) + $(4 \times meta \ corr)$			$C_{r}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = 0$	-536.10	-543.20 266.41 309.94 -1008.55	7.10	64COL/PER
Li	iterature – Calculated	= Residual	Reference	$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = $		- 242.50 97.82		
Gas phase $\Delta_t H^\circ =$ Liquid phase	-421.95		·.	(1×O-(I (1×CO-	$I(C_B) + (1$; Salicylic acid $1 \times C_B - (O) + (1 \times O - (H)) + (O)$ to corr)	$1 \times C_{B}$ -(CO))	
$\Delta_t H^\circ = C_p^\circ =$	-507.74 313.37					re – Calculated	= Residual	Reference
$C_p^{\circ} =$	06.10 - 515.83 242.35	9.73	64COL/PER	Gas phase $\Delta_t H^\circ =$	- 494.80	-493.61	-1.19	54DAV/JON
$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$	281.50 - 900.68 - 247.29 99.76			Liquid phas $\Delta_t H^\circ = C_p^\circ =$	se	- 579.86 265.44		
$(3 \times C_B - (H))(0)$	oic acid C)) + $(2 \times C - (H)_2(C)(C \times C_B)_2$) + $(1 \times C_B - (CO))$ CO)) + $(3 \times meta \ corr)$			$C_{\rho}^{\circ} = S^{\circ} =$	589.90	-591.13 154.94 175.20	1.23	35STI/HUF
L	iterature - Calculated	= Residual	Reference	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-564.26 -422.90 170.59		
Gas phase $\Delta_t H^\circ = -40$	07.80 -404.18	-3.62	74ROU/TUR	(2×O-(I	1)(CO))+(lic acid; Phthal (2×CO-(O)(C ₁ (1×COOH-C	$(2 \times C_B - ($	
Liquid phase $\Delta_t H^\circ = C_p^\circ =$	-497.18 297.37					'alculated = Res		
Solid phase	11.90 - 503.29 292.99 278.42 - 903.76 - 233.83 94.33	-8.61	74ROU/TUR	Solid phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{\ell}S^{\circ} = \Delta_{\ell}G^{\circ} = \ln K_{\ell} =$	- 782.07 188.11 207.94	- 777.74 186.44 207.94 - 639.78 - 586.99 236.79	-4.33 1.67 0.00	61SCH/WAG 36PAR/TOD 36PAR/TOD

Table 19. Acids (89) - Continued

$(4 \times C_B - (H)$	(CO)) + $(2 \times CC)$ $(C_B)_2$) + $(1 \times CC)$				$(3\times C_B-(H)(C_B)_2)$	+(3×00011-0	OOII (meta cc	orr))
	Literature – C	alculated=	Residual	Reference	Literat	ure – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = -$	696.30 - 0	696.30	0.00	62KRA/BER	Gas phase $\Delta_t H^\circ =$	- 1121.79		
Solid phase					Solid phase			
•	803.00 -	798.74	- 4.26	71YUK/BIK	$\Delta_{\rm f}H^{\circ} = -1190.10$	-1197.99	7.89	71YUK/BIK
$C_p^{\circ} =$	201.70	201.44	0.26	39SAT/SOG2	$C_p^{\circ} =$	286.77		
S° =		198.98			S° =	230.22		
$\Delta_f S^o =$		648.74			$\Delta_{\rm f} S^{\circ} =$	-828.28		
$\Delta_f G^\circ =$		605.32			$\Delta_i G^{\circ} =$	- 951.04		
$lnK_f =$		244.18 			$lnK_f =$	383.64		T
(4×C _B -(H	Literature – (Calculated =	= Residual	Reference	(1×CO-(O)(C _B))	ure – Calculated		Reference
Gas phase $\Delta_t H^\circ = -$	717.90 -	672.36	- 45.54	34HIR	Gas phase $\Delta_t H^\circ = -223.10$	-226.93	3.83	74COL/ROU
$C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} - \Delta_{t}G^{\circ}$	- -816.18 – -	797.64 271.46 811.88 171.44 198.98 648.74 618.46 249.48	4.30	71YUK/BIK	Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ Solid phase $\Delta_{t}H^{\circ} = 333.50$ $C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = $	-326.36 268.17 -345.09 190.97 201.24 -589.23 169.41 68.34	11.59	74COL/ROU
$lnK_{\ell} =$		- 43		a w o	A March divide and A			a
1,2,3-Benzene (3×O-(H) (3×C _B -(H) (1×COOF	e tricarboxylic ()(CO)) + (3 × C ()(C _B) ₂) + (2 × c H-COOH (met	CO-(O)(C _B) COOH-CO (a corr))	OOH (onho c	orr))+	2-Naphthoic acid (7 × C _B -(H)(C _B) ₂)· (1 × CO-(O)(C _B))· Literate)))	$C_{11}H_{g}$ C_{H} C_{H} C_{H}
1,2,3-Benzene (3×O-(H) (3×C _B -(H) (1×COOF	$(CO) + (3 \times C)$ $(C_B)_2 + (2 \times C)$	CO-(O)(C _B) COOH-CO (a corr))	OOH (onho c	CO)(C _B) ₂) + orr)) +	$(7 \times C_B - (H)(C_B)_2)$ $(1 \times CO - (O)(C_B))$ Literate	+ (1×O-(H)(CC)))	(CO))+
1,2,3-Benzen (3×O-(H) (3×C _B -(H) (1×COOH Lite:)(CO)) + (3 × C f)(C _B) ₂) + (2 × H-COOH (met rature-Calcula	CO-(O)(C _B) COOH-CO (a corr)) ted = Reside	OOH (<i>onho</i> co	CO)(C _B) ₂) + orr)) +	$(7 \times C_B - (H)(C_B)_2) \cdot (1 \times CO - (O)(C_B))$	+ (1×O-(H)(CC)))	' _в -(CO)) +
1,2,3-Benzen $(3 \times O - (H))$ $(3 \times C_B - (H))$ $(1 \times COOH)$ Lite: Solid phase $\Delta_l H^{\circ} = -11$	(CO)) + (3 × C f)(C _B) ₂) + (2 × c H-COOH (met rature-Calcula)	CO-(O)(C _B) COOH-CO ra corr)) ted = Reside	OOH (onho c	CO)(C _B) ₂) + orr)) +	$(7 \times C_B - (H)(C_B)_2)$ $(1 \times CO - (O)(C_B))$ Literate	+ (1 × O-(H)(CC ure – Calculated	= Residual	Reference
1,2,3-Benzen (3 × O-(H) (3 × C _B -(H) (1 × COOH Liter Solid phase $\Delta_t H^\circ = -11$ $C_\rho^\circ =$	(CO)) + (3 × C f)(C _B) ₂) + (2 × c H-COOH (met rature-Calcular	CO-(O)(C _B) COOH-CO (a corr)) ted = Resident 155.99 256.77	OOH (<i>onho</i> co	CO)(C _B) ₂) + orr)) +	$(7 \times C_B - (H)(C_B)_2)$ $(1 \times CO - (O)(C_B))$ Literate Gas phase $\Delta_t H^\circ = -232.50$	+ (1 × O-(H)(CC ure – Calculated	= Residual	Reference
1,2,3-Benzene $(3 \times O - (H))$ $(3 \times C_B - (H))$ $(1 \times COOH)$ Literative Solid phase $\Delta_t H^{\circ} = -11$ $C_{\rho}^{\circ} =$ $S^{\circ} =$	(CO)) + (3 × C f)(C _B) ₂) + (2 × c H-COOH (met rature-Calcular	CO-(O)(C _B) COOH-CO (a corr)) ted = Reside 155.99 256.77 248.14	OOH (<i>onho</i> co	CO)(C _B) ₂) + orr)) +	$(7 \times C_B - (H)(C_B)_2)$ $(1 \times CO - (O)(C_B))$ Literate Gas phase $\Delta_t H^\circ = -232.50$ Liquid phase	+ (1 × O-(H)(CC) ure – Calculated - 226.93	= Residual	Reference
1,2,3-Benzen (3 × O-(H) (3 × C _B -(H) (1 × COOH Liter Solid phase $\Delta_t H^\circ = -11$ $C_\rho^\circ =$	(CO)) + (3 × C (CB) ₂) + (2 × c H-COOH (men rature-Calcula 160.30 - 1	CO-(O)(C _B) COOH-CO (a corr)) ted = Resident 155.99 256.77	OOH (<i>onho</i> co	CO)(C _B) ₂) + orr)) +	$(7 \times C_B - (H)(C_B)_2)$ $(1 \times CO - (O)(C_B))$ Literate Gas phase $\Delta_t H^\circ = -232.50$	+ (1 × O-(H)(CC ure – Calculated	= Residual	Reference

2-Naphthoic acid (Continued) $C_{11}H_8O_2$ $(7 \times C_B-(H)(C_B)_2) + (2 \times C_{BF}-(C_{BF})(C_B)_2) + (1 \times C_B-(CO)) + (1 \times CO-(O)(C_B)) + (1 \times O-(H)(CO))$	racemic-2,3-Diphenylbutandedioic acid; racemic-2,3-Diphenylsuccinic acid $(2\times O-(H)(CO)) + (2\times CO-(C)(O)) + (2\times C-(H)(CO)) + (2\times C_B-(C)(C_B)_2) + (10\times C_B-(H)(C_B)_2)$	C ₁₆ H ₁₄ O ₄ CO)(C)(C _B)) +
Literature - Calculated = Residual Reference	Literature-Calculated = Residual	Reference
Solid phase $\Delta_t H^\circ = -346.10 -345.09 -1.01$ 74COL/ROU $C_p^\circ = 190.97$	Solid phase $\Delta_t H^\circ = -740.10 -748.78 8.68$	33VER/HAR
$S^{\circ} = 201.24$ $\Delta_{f}S^{\circ} = -589.23$ $\Delta_{f}G^{\circ} = -169.41$ $\ln K_{f} = 68.34$	$ \begin{array}{l} \textbf{2-Methoxybenzoic acid} \\ (4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (CO)(C_B)_2) + (1 \times C_B -$	(C _B))+
3-Hydroxy-2-naphthoic scid C ₁₁ H ₈ O ₃	Literature - Calculated = Residual	Reference
3-Hydroxy-2-naphthoic acid $C_{11}H_8O_3$ $(1 \times O - (H)(C_B)) + (1 \times O - (H)(CO)) + (1 \times CO - (O)(C_B)) + (1 \times C_B - (CO)) + (1 \times C_B - (II)(C_B)_2) + (2 \times C_{BF} - (C_{BF})(C_B)_2) + (1 \times OH - COOH (ortho corr))$	Gas phase $\Delta_t H^\circ = -433.80 -433.12 -0.68$	78COL/JIM
Literature - Calculated = Residual Reference	Solid phase $\Delta_t H^\circ = -538.50 -538.49 -0.01$	78COL/JIM
Gas phase $\Delta_t H^\circ = -425.79$		
Liquid phase $\Delta_t H^\circ = -531.88$ $C_p^\circ - 329.84$	3-Methoxybenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (CO)(C_B)_2) + (1 \times C_B - (CO)(C_B)_2) + (1 \times O - (C)(C_B)) + (1 \times O - (H)(CO)) + (1 \times O - (C)(C_B)) + (1 \times C - (H)_3(O)) + (1 \times C + (H)_3 - COOH (meta corr))$ Literature – Calculated = Residual	
Solid phase $\Delta_t H^\circ = -547.80 -549.87$ 2.07 56YOU/KEI $C_p^\circ = 199.80$ $S^\circ = 208.70$	Gas phase $\Delta_l H^\circ = -446.10 -443.12 -2.98$	78COL/JIM
$\Delta_t S^\circ = -684.29$ $\Delta_t G^\circ = -345.85$ $\ln K_\ell = 139.51$	Solid phase $\Delta_t H^\circ = -553.50 -556.49$ 2.99	78COL/JIM
$\label{eq:continuous} \begin{split} & \textbf{Phenylbutanedioic acid; Phenylsuccinic acid} & \textbf{C}_{10}\textbf{H}_{10}\textbf{O}_4 \\ & (2\times O-(H)(CO)) + (2\times CO-(C)(O)) + (1\times C-(H)_2(CO)(C)) + \\ & (1\times C-(H)(CO)(C)(C_B)) + (1\times C_B-(C)(C_B)_2) + (5\times C_B-(H)(C_B)_2) \end{split}$	$ \label{eq:acid} \begin{array}{l} \textbf{4-Methoxybenzoic acid} \\ (4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (CO)(C_B)_2) + (1 \times C_B - (CO)(C_B)$	
Solid phase $\Delta_t H^\circ = -841.00 - 838.04 - 2.96$ 33VER/HAR	Literature - Calculated = Residual	Reference
meso-2,3-Diphenylbutanedioic acid; meso-	Gas phase $\Delta_t H^{\circ} = -451.90 -448.12 -3.78$	78COL/JIM
2,3-Diphenylsuccinic acid $C_{16}H_{14}O_4$ $(2 \times O-(H)(CO)) + (2 \times CO-(C)(O)) + (2 \times C-(H)(CO)(C)(C_B)) +$ $(2 \times C_B-(C)(C_B)_2) + (10 \times C_B-(H)(C_B)_2)$ Literature-Calculated = Residual Reference	Liquid phase $\Delta_t H^\circ = -540.57$ $C_p^\circ = 265.38$	
Solid phase $\Delta_t H^{\circ} = -733.50 -748.78$ 15.28 33VER/HAR	Solid phase $\Delta_e H^\circ = -561.70 - 561.49 - 0.21$	78COL/JIM

TABLE 20. Anhydrides (11)

TABLE 20. Anhydrides (11) - Continued

(170-($H)_3(C)) + (2)$	tetic anhydride $< CO-(C)(O)$ tic), $\sigma = 18$		C ₄ H ₆ O ₃	(2×C-(H				nued) C ₄ H ₄ O (CO) ₂ , aliphatic) +
	Literatur	e – Calculated	- Residual	Reference		Literatur	e – Calculated -	- Residual	Reference
Gas phase $H^{\circ} = C_{p}^{\circ} =$	- 573.50 99.50	-573.50 99.50	0.00 0.00	47STU 69STU/WES	Liquid phase $\Delta_t H^\circ =$		-588.60	0.00	13TAM
$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = 0$	389.95	389.95 -332.29 -474.43 191.38	0.00	69STU/WES	Solid phase $\Delta_t H^\circ =$	608.60	-608.60	0.00	90YAN/PIL
Liquid phate $\Delta_t H^\circ = C_p^\circ =$	ase - 624.40 168.20	-624.46 168.20	0.06 0.00	62WAD 62WAD		$I_{2}(C)_{2}+(2$	2×C-(H)₂(CO)e atic) + (1×Gluta		
						Literatu	e – Calculated =	Residual	Reference
(2×C-(Propionic anhy × C-(H)2(CO) tic)		C ₆ H ₁₀ O ₃ O-(C)(O)) +	Gas phase $\Delta_t H^\circ =$	-532.40	-532.40	0.00	90YAN/PIL
	Literatur	e – Calculated	= Residual	Reference	Solid phase				
Gas phase $A_tH^\circ = C_p^\circ =$	- 626.51	-617.18 148.88	- 9.33	47STU		-618.50	- 618.50 	0.00	90YAN/PIL
Liquid phate $\Delta_i H^\circ = C_p^\circ =$	ase 679.10	- 672.74 226.78	- 6.36	42CON/KIS	(2×CO-	(C)(C) + (1)(C)(C) + (1)(C)(C) + (1)(C)(C) + (1)(C)(C) + (1)(C)(C) + (1)(C)(C)(C) + (1)(C)(C)(C) + (1)(C)(C)(C) + (1)(C)(C)(C) + (1)(C)(C)(C) + (1)(C)(C)(C) + (1)(C)(C)(C)(C) + (1)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)	× C–(H)(CO)(C 1 × O–(CO) ₂ , ali ary)) + (1 × Succ	phatic) + cinic anhydric	le rsc)
						Literatui	e – Calculated =	Residual	Reference
(6×C-($(H)_3(C)) + (6$	anhydride; Pi ×-CH ₃ corr (o (2×CO-(C)(O	quaternary))+	•	Gas phase $\Delta_t H^\circ =$	makat kat kat kat mayana manan	-550.83		
	Literatur	re – Calculated	= Residual	Reference	Liquid phas $\Delta_t H^\circ =$		-618.14	0.54	42CON/KIS
Gas phase Δ _t H° =	e	722.04			Solid phase	-620.00	-639.61	19.61	33VER/HAR
$\Delta_i H^{\circ} =$		-722.04 -788.94 330.10	8.94	42CON/KIS	Solid phase $\Delta_t H^\circ =$ 2,2-Dimethy $(2 \times C - (1 \times C) - (2 \times C) - (2 \times C) - (2 \times C) - (2 \times C)$	-620.00 ylsuccinic a H) ₃ (C))+(1 (C)(O))+(**	nhydride × C-(CO)(C) ₃)· I × O-(CO) ₂ , ali	+ (1 × C-(H) ₂	C ₆ H ₈ O ₂ (CO)(C))+
Liquid ph $\Delta_t H^\circ = C_p^\circ =$ Dihydrofu $(2 \times C - ($	ase - 780.00 aran-2,5-dion	-788.94 330.10 e; Succinic ant +(2×CO-(C)	hydride	42CON/KIS C ₄ H ₄ O ₃ -(CO) ₂ , aliphatic) +	Solid phase $\Delta_t H^\circ =$ 2,2-Dimethy $(2 \times C - (1 \times C) - (2 \times C) - (2 \times C) - (2 \times C) - (2 \times C)$	-620.00 ylsuccinic a H) ₃ (C))+(1 (C)(O))+(3 corr (quant	nhydride × C-(CO)(C) ₃)	+ (1 × C-(H) ₂ phatic) + Succinic anhy	C ₆ H ₈ O (CO)(C))+

-527.90

0.00

90YAN/PIL

Gas phase $\Delta_i H^\circ = -527.90$

TABLE 20. Anhydrides (11) - Continued

TABLE 20. Anhydrides (11) - Continued

2,2-Dimethylsuccinic anhydride (Continued)	$C_6H_8O_3$
$(2 \times C - (H)_3(C)) + (1 \times C - (CO)(C)_3) + (1 \times C - (H)_2(CO)(C))$	+
$(2 \times CO-(C)(O)) + (1 \times O-(CO)_2$, aliphatic) +	
(2×-CH ₃ corr (quaternary)) + (1×Succinic anhydride rsc)	

Literatur	Literature – Calculated = Residual				
Liquid phase $\Delta_t H^{\circ} = -645.50$	- 642.31	-3.19	42CON/KIS		
Solid phase $\Delta_t H^\circ = -651.50$	- 658.86	7.36	33VER/HAR		

Tetramethylsuccinic anhydride

C₈H₁₂O₃

 $(4 \times C-(H)_3(C))+(4 \times -CH_3 \text{ corr (quaternary)})+$ $(2 \times C-(CO)(C)_3)+(2 \times CO-(C)(O))+(1 \times O-(CO)_2, \text{ aliphatic})+$ $(1 \times Succinic \text{ anhydride rsc})$

Lit	Literature – Calculated = Residual		
Gas phase Δ _t H° =	- 623.64		
Liquid phase Δ _t H° =	- 696.02		
Solid phase $\Delta_t H^\circ = -712$	2.80 - 709.12	-3.68	33VER/HAR

2,2-Diethylsuccinic anhydride

 $C_8H_{12}O_3$

 $(2 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)_2) + (1 \times C - (CO)(C)_3) + (1 \times C - (H)_2(CO)(C)) + (2 \times CO - (C)(O)) + (1 \times O - (CO)_2$, aliphatic) + $(1 \times Succinic anhydride rsc)$

L	Literature – Calculated = Residual			
Gas phase Δ _t H° =	- 607.91			
Liquid phase Δ _t H° =	- 684.99			
Solid phase $\Delta_t H^\circ = -68$	38.80 - 708.98	20.18	33VER/HAR	

Benzoic anhydride	C14H10O3
$(10 \times C_B - (H)(C_B)_2) + (2 \times C_B - (CO)(C_B)_2) + (2 \times CO - (O)(C_B)_2)$	(C_B)) +
$(1 \times O - (CO)_2$, aromatic)	

Literatu	Literature – Calculated = Residual			
Gas phase $\Delta_t H^\circ = -319.23$	-319.20	-0.03	71CAR/FIN	
Liquid phase $\Delta_t H^\circ = -398.32$	-398.30	-0.02	71CAR/FIN	
Solid phase $\Delta_t H^\circ = -415.47$	- 415.40	- 0.07	71CAR/FIN	

Phthalic anhydride $\begin{array}{l} C_8H_4O_3\\ (4\times C_B-(H)(C_B)_2)+(2\times C_B-(CO)(C_B)_2)+(2\times CO-(O)(C_B))+\\ (1\times O-(CO)_2,\ aromatic)+(1\times Phthalic\ anhydride\ rsc) \end{array}$

Literatu	re – Calculated =	Reference	
Gas phase $\Delta_f H^\circ = -371.40$	-371.40	0.00	46CRO/FEE
Solid phase $\Delta_t H^{\circ} = -460.10$	- 460.10	0.00	50PAR/MOS

TABLE 21. Esters (74)

<u>.</u>	Literatur	Literature - Calculated - Residual				
Gas phase	•					
$\Delta_t H^{\circ} =$	-355.50	-355.52	0.02	71HAL/BAL		
$C_p^{\circ} =$	66.53 301.25	66.53	0.00	69STU/WES		
S° =	301.25	301.25	0.00	69STU/WES		
$\Delta_f S^{\circ} =$		-176.42				
$\Delta_f G^{\circ} =$		-302.92				
$lnK_f =$	·	122.20				
Liquid ph	ase					
	-386.10	-386.05	-0.05	71HAL/BAL		
$C_p^{\circ} =$	119.66	121.16	- 1.50	79FUC		
s° =		216.26				
$\Delta_f S^\circ =$		-261.40				
$\Delta_f G^{\circ} =$		-308.11				
$lnK_f =$		124.29	-			
Methyl et	hanoate; Me	thyl acetate		C ₃ H ₆ C		

	Literatur	Reference		
Gas phase				
$\Delta_{\rm f}H^{\circ} =$	-410.00	-410.63	0.63	71HAL/BAL
$C_p^{\circ} =$		87.82		
Liquid photostate $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S$		-440.61 137.52 237.60 -376.38 -328.39	-5.19 -13.67	71HAL/BAL 71HAL/BAL

Methyl propanoate; Methyl propionate $C_4H_8O_2\\ (2\times C-(H)_3(C))+(1\times C-(H)_2(CO)(C))+(1\times CO-(C)(O))+\\ (1\times O-(C)(CO))$

	Literature – Calculated = Residual			Reference	
Gas phase					
$\Delta_t H^{\circ} =$		-432.47			
$C_p^{\circ} =$		112.51			
T::					
Liquid pha $\Delta_t H^\circ =$		-464.75			
$\Delta_f H^\circ = C_p^\circ =$	se 174.05	166.81	7.24	79FUC	
$\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} =$			7.24	79FUC	
$\Delta_f H^\circ = C_p^\circ =$		166.81	7.24	79FUC	
$\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} =$		166.81 277.47	7.24	79FUC	

(2×C-(H	Methyl butanoate; Methyl butyrate $(2 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) - (1 \times CO (C)(O)) + (1 \times O (C)(CO))$				
,	Literature – Calculated = Residual	Reference			
Gas phase		- 1			
$\Delta_{\mathbf{f}}H^{\hat{\circ}} =$	-453.10				
$C_n^{\circ} =$	135.40				

$\Delta_{f}H^{\circ} = C_{p}^{\circ} =$		-453.10 135.40		
Liquid pha	nea.			
$\Delta_t H^\circ =$	isc	- 490.48		
$C_p^{\circ} =$	200.83	197.23	3.60	79FUC
S° =		309.85	-,	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
$\Delta_{\mathbf{f}}S^{\circ} =$		-576.75		
$\Delta_t G^\circ =$		-318.52		
$lnK_f =$		128.49		

 $\label{eq:condition} \begin{array}{ll} \text{Methyl pentanoate; Methyl valerate} & C_6H_{12}O_2\\ (2\times C-(H)_3(C)) + (2\times C-(H)_2(C)_2) + (1\times C-(H)_2(CO)(C)) + \\ (1\times CO-(C)(O)) + (1\times O-(C)(CO)) \end{array}$

	Literatui	Reference			
Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 471.10	-473.73 158.29	2.63	77MAN/SEL	
Liquid ph					
$\Delta_{\epsilon}H^{\circ} =$	-514.20	-516.21	2.01	65ADR/DEK	
	229.28	227.65	1.63	79FUC	
$C_n^n =$					
$C_p^{\circ} = S^{\circ} =$		342.23			
		342.23 - 680.68			
<i>S</i> ° =					

 $\label{eq:condition} \begin{array}{ll} \text{Methyl hexanoate; Methyl caproate} & C_7H_{14}O_2\\ (2\times C-(H)_3(C)) + (3\times C-(H)_2(C)_2) + (1\times C-(H)_2(CO)(C)) + \\ (1\times CO-(C)(O)) + (1\times O-(C)(CO)) \end{array}$

	Literatu	Reference		
Gas phase	e			
$\Delta_{\rm f}H^{\circ} =$	-492.20	-494.36	2.16	77MAN/SEL
$C_r^{\circ} =$		181.18		
Liquid ph $\Delta_t H^\circ =$		-541.94	1.74	65ADR/DEK
		- 541.94 258.07	1.74	65ADR/DEK
$\Delta_t H^\circ =$			1.74	65ADR/DEK
$\Delta_t H^\circ = C_p^\circ =$		258.07	1.74	65ADR/DEK
$\Delta_t H^\circ = C_p^\circ = S^\circ =$		258.07 374.61	1.74	65ADR/DEK

TABLE 21. Esters (74) - Continued

(2×C-(H	$(1)_3(C) + (4)$	ethyl enanthate × C-(H) ₂ (C) ₂) - t × O-(C)(CO))	+ (1 × C-(H) ₂ (C ₈ H ₁₆ O ₂ (CO)(C))+	(2×C-(I	1)3(C))+(7	thyl caprate '×C-(H) ₂ (C) ₂)- 1×O-(C)(CO)		C ₁₁ H ₂₂ O (CO)(C)) +
	Literatur	e – Calculated =	= Residual	Reference		Literatu	re – Calculated :	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	-515.50	514.99 204.07	-0.51	77MAN/SEL	Gas phase $\Delta_t H^\circ = C_\rho^\circ =$	-573.80	576.88 272.74	3.08	77MAN/SEL
Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = S^\circ =$	se - 567.10 285.10	- 567.67 288.49 406.99 - 888.54 - 302.75 122.13	0.57 -3.39	65ADR/DEK 79FUC	Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se - 640.50 382.80	-644.86 379.75 504.13 -1200.33 -286.98 115.77	4.36 3.05	65ADR/DEK 79FUC
(2×C-(F	I) ₃ (C))+(5 (C)(O))+(hyl caprylate ×C-(H) ₂ (C) ₂)- 1×O-(C)(CO))		(2×C-(F	·H)₃(C)) + (8 ·(C)(O)) + (Methyl undecyla × C-(H) ₂ (C) ₂)- 1 × O-(C)(CO)) re – Calculated =	+ (1 × C-(H) ₂	
	Literatui	re – Calculated : –––––	= Residual	Reference		Literatu	re – Calculated =	= Kesiduai	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	-533.90	-535.62 226.96	1.72	77MAN/SEL	Gas phase $\Delta_t H^\circ = C_p^\circ =$	-593.80	-597.51 295.63	3.71	77MAN/SEL
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	se 590.30	- 593.40 318.91 439.37 - 992.47 - 297.49 120.01	3.10	65ADR/DEK	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se 665.20	-670.59 410.17 536.51 -1304.27 -281.72 113.65	5.39	65ADR/DEK
(2×C-(I	$(H)_3(C)) + (6)$	ethyl perlargons i× C-(H) ₂ (C) ₂) 1× O-(C)(CO)	$+(1\times C-(H)_2$	C ₁₆ H ₂₆ O ₂ (CO)(C)) +	(2×C-(I	f(C) + (9)	Methyl laurate × C-(H) ₂ (C) ₂) - 1 × O-(C)(CO))		C ₁₃ H ₂₆ O ₂ (CO)(C))+
	Literatu	re – Calculated	= Residual	Reference		Literatu	re – Calculated = 	= Residual	Reference
Gas phase $\Delta_l H^\circ = C_p^\circ =$	-554.20	- 556.25 249.85	2.05	77MAN/SEL	Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 615.90	-618.14 318.52	2.24	77MAN/SEL
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se -616.20	- 619.13 349.33 471.75 - 1096.40 - 292.24 117.89	2.93	65ADR/DEK	Liquid phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se 693.00	- 696.32 440.59 568.89 - 1408.20 - 276.47 111.52	3.32	65ADR/DEK

TABLE 21. Esters (74) - Continued

(2×C-(H		\times C-(H) ₂ (C) ₂) \times O-(C)(CO))	+ (1 × C-(H)	₂ (CO)(C))+			×O-(C)(CO) (1×CO-(C)((CO)(C))+
·	Literature	- Calculated =	Residual	Reference		Literatur	re – Calculated	d = Residual	Reference
Gas phase '' $\Delta_t H^\circ = C_p^\circ =$	- 635.30	-638.77 341.41	3.47	77MAN/SEL	Gas phase $\Delta_l H^\circ = C_p^\circ =$		-700.66 410.08		
Liquid phas	ie			i ^{to} P	Liquid pha	se			
$\Delta_i H^\circ =$	-717.90	-722.05	4.15	65ADR/DEK	$\Delta_t H^\circ =$		- 799.24		
$C_p^{\circ} =$		471.01			$C_p^{\circ} =$		562.27		
s° -		601.27			S° -		698.41		
$\Delta_f S^\circ =$		-1512.13		1	$\Delta_{f}S^{\circ} =$		-1823.92		
$\Delta_t G^{\circ} =$		-271.21			$\Delta_t G^\circ =$		-255.44		
$lnK_t =$		109.40			$lnK_f =$		103.04		
					Solid phase	;			
Methyl tetra	adecanoate;	Methyl myrista	ate	$C_{15}H_{30}O_2$	$\Delta_i H^\circ =$		-867.91		
(2×C-(I	I)₃(C)) + (11	\times C-(H) ₂ (C) ₂)	+ (1 × C-(H)	₂ (CO)(C))+	$C_p^{\circ} =$	474.47	480.76	-6.29	56WIR/DRO
(1×CO-	(C)(O))+(1	×0-(C)(CO))			S° =	495.09	481.46	13.63	56WIR/DRO
					$\Delta_{\mathbf{f}}S^{\circ} =$		- 2040.87		
	Literature	e – Calculated =	= Residual	Reference	$\Delta_{l}G^{\circ} =$		- 259.42		
					$lnK_f =$		104.65		
Gas phase $\Delta_t H^\circ =$	- 656.90	-659.40	2.50	77MAN/SEL	Ethyl meth	anoate; Eth	yl formate		C ₃ H ₆ O ₂
•	-656.90	-659.40 364.30	2.50	77MAN/SEL		(C) + (1)		C))+(1×O-(0	C ₃ H ₆ O ₂
$\Delta_t H^{\circ} = C_p^{\circ} =$ Liquid phase	se	364.30		·	(1 × C-(I	1) ₃ (C)) + (1 (H)(O))			
$\Delta_t H^\circ = C_p^\circ = $ Liquid phas $\Delta_t H^\circ = $	se -743.90	364.30 -747.78	3.88	65ADR/DEK	(1 × C-(I	1) ₃ (C)) + (1 (H)(O))	× C-(H) ₂ (O)(C)(CO))+
$\Delta_t H^\circ = C_p^\circ = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = $	se	-747.78 501.43		·	(1×C-(I (1×CO-	1) ₃ (C)) + (1 (H)(O))	× C-(H) ₂ (O)(C)(CO))+
$\Delta_t H^{\circ} = C_p^{\circ} = $ Liquid phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = $	se -743.90	-747.78 501.43 633.65	3.88	65ADR/DEK	(1×C-(I (1×CO-	1) ₃ (C)) + (1 (H)(O))	× C-(H) ₂ (O)(C)(CO))+
$\Delta_t H^{\circ} = C_p^{\circ} =$ Liquid phas $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} =$	se -743.90	-747.78 501.43 633.65 -1616.06	3.88	65ADR/DEK	$(1 \times C - (H \times C) - (H \times C) - (H \times C)$ Gas phase $\Delta_t H^\circ = (H \times C)$	1) ₃ (C)) + (1 (H)(O))	× C-(H) ₂ (O)(re - Calculatec - 388.42		C)(CO))+
$\Delta_t H^{\circ} = C_p^{\circ} = $ Liquid phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = $	se -743.90	-747.78 501.43 633.65	3.88	65ADR/DEK	(1×C-(I (1×CO-	1) ₃ (C)) + (1 (H)(O))	× C-(H) ₂ (O)(C)(CO))+
$\Delta_t H^\circ = C_p^\circ = C_p^\circ = C_p^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = C_p^\circ = $	se -743.90	-747.78 501.43 633.65 -1616.06 -265.95	3.88	65ADR/DEK	$(1 \times C - (H + C) - (1 \times C) - (1 \times C) - (1 \times C)$ Gas phase $\Delta_t H^\circ = C_p^\circ =$	1) ₃ (C)) + (1 (H)(O)) Literatur	× C-(H) ₂ (O)(re - Calculated - 388.42 86.86		C)(CO))+
$\Delta_t H^{\circ} = C_P^{\circ} = C_P^{\circ} = C_P^{\circ} = C_P^{\circ} = C_P^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = C_L^{\circ} = C_$	se - 743.90 505.40	-747.78 501.43 633.65 -1616.06 -265.95 107.28	3.88 3.97	65ADR/DEK 79FUC	$(1 \times C - (H + C) - (1 \times C) - (1 \times C) - (1 \times C)$ Gas phase $\Delta_t H^\circ = C_p^\circ = - (1 \times C)$ Liquid phase $\Delta_t H^\circ = - (1 \times C)$	H ₃ (C)) + (1 (H)(O)) Literatur	× C-(H) ₂ (O)(re - Calculated - 388.42 86.86 - 421.85	i = Residual	C)(CO)) + Reference
$\Delta_t H^{\circ} = C_t^{\circ} = C_t^{\circ} = C_t^{\circ} = C_t^{\circ} = C_t^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = InK_f = Methyl pen$	se - 743.90 505.40	-747.78 501.43 633.65 -1616.06 -265.95 107.28	3.88 3.97 decylate	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $	1) ₃ (C)) + (1 (H)(O)) Literatur	× C-(H) ₂ (O)(re - Calculated - 388.42 86.86 - 421.85 154.80		C)(CO))+
$\Delta_t H^{\circ} = C_r^{\circ} = $ Liquid phas $\Delta_t H^{\circ} = C_r^{\circ} = S^{\circ} = \Delta_t G^{\circ} = InK_t = $ Methyl pen (2×C-(I	se - 743.90 505.40 stadecanoate	-747.78 501.43 633.65 -1616.06 -265.95 107.28 :; Methyl penta 2×C-(H) ₂ (C) ₂)	3.88 3.97 decylate + (1 × C-(H)	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ Liquid phas $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ $S^{\circ} = $	H ₃ (C)) + (1 (H)(O)) Literatur	× C-(H) ₂ (O)(re - Calculated - 388.42 86.86 - 421.85 154.80 248.85	i = Residual	C)(CO)) + Reference
$\Delta_t H^{\circ} = C_r^{\circ} = $ Liquid phas $\Delta_t H^{\circ} = C_r^{\circ} = S^{\circ} = \Delta_t G^{\circ} = InK_t = $ Methyl pen (2×C-(I	se - 743.90 505.40 stadecanoate	-747.78 501.43 633.65 -1616.06 -265.95 107.28	3.88 3.97 decylate + (1 × C-(H)	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ Liquid phas $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ $S^{\circ} = \Delta_{t}S^{\circ} = $	H ₃ (C)) + (1 (H)(O)) Literatur	- 388.42 86.86 - 421.85 154.80 248.85 - 365.13	i = Residual	C)(CO)) + Reference
$\Delta_t H^{\circ} = C_t^{\circ} = C_t^{\circ} = C_t^{\circ} = C_t^{\circ} = C_t^{\circ} = S^{\circ} = \Delta_t G^{\circ} = InK_t = Methyl pen (2 × C - (I$	se - 743.90 505.40 stadecanoate H ₃ (C)) + (12 (C)(O)) + (13	-747.78 501.43 633.65 -1616.06 -265.95 107.28 :; Methyl penta 2×C-(H) ₂ (C) ₂)	3.88 3.97 decylate + (1 × C-(H)	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ Liquid phas $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ $S^{\circ} = $	H ₃ (C)) + (1 (H)(O)) Literatur	× C-(H) ₂ (O)(re - Calculated - 388.42 86.86 - 421.85 154.80 248.85	i = Residual	C)(CO)) + Reference
$\Delta_t H^{\circ} = C_P^{\circ} = C_P^{\circ} = C_P^{\circ} = C_P^{\circ} = C_P^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = InK_t = Methyl pen (2 \times C - (I \times CO - I))$	se - 743.90 505.40 stadecanoate H ₃ (C)) + (12 (C)(O)) + (13	-747.78 501.43 633.65 -1616.06 -265.95 107.28 c; Methyl penta 2×C-(H) ₂ (C) ₂) 1×O-(C)(CO))	3.88 3.97 decylate + (1 × C-(H)	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂ O ₂ (CO)(C)) +	Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phas $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t G^\circ = \Delta_t G^\circ = \ln K_t =$	H ₃₃ (C)) + (1 (H)(O)) Literatur Se 144.35	- 421.85 154.80 248.85 - 365.13 - 312.99 126.26	i = Residual	Reference 79FUC
$\Delta_t H^{\circ} = C_P^{\circ} = C_P^{\circ} = C_P^{\circ} = C_P^{\circ} = C_P^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = InK_t = Methyl pen (2 \times C - (1 \times CO - C))$	se -743.90 505.40 stadecanoate H ₃ (C))+(12 (C)(O))+(13 Literatur	364.30 -747.78 501.43 633.65 -1616.06 -265.95 107.28 c; Methyl penta 2 × C-(H) ₂ (C) ₂) 1 × O-(C)(CO)) e - Calculated =	3.88 3.97 decylate + (1 × C-(H)	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂ O ₂ (CO)(C)) + Reference	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $\Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} =$ $\ln K_{t} =$ Ethyl ethan	H ₃₃ (C)) + (1 (H)(O)) Literatur se 144.35	- 421.85 154.80 248.85 - 365.13 - 312.99 126.26	1 = Residual - 10.45	C)(CO)) + Reference 79FUC
$\Delta_t H^{\circ} = C_P^{\circ} = C_P^{\circ} = C_P^{\circ} = C_P^{\circ} = C_P^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = InK_t = Methyl pen (2 \times C - (I \times CO - I))$	se - 743.90 505.40 stadecanoate H ₃ (C)) + (12 (C)(O)) + (13	-747.78 501.43 633.65 -1616.06 -265.95 107.28 c; Methyl penta 2×C-(H) ₂ (C) ₂) 1×O-(C)(CO))	3.88 3.97 decylate + (1 × C-(H)	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂ O ₂ (CO)(C)) +	Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ = \ln K_t =$ Ethyl ethan $(2 \times C - (H + L))$	H ₃₃ (C)) + (1 (H)(O)) Literatur se 144.35	- 421.85 154.80 248.85 - 365.13 - 312.99 126.26	i = Residual	C)(CO)) + Reference 79FUC
$\Delta_t H^\circ = C_\rho^\circ = C_\rho^\circ = C_\rho^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t = $	se -743.90 505.40 stadecanoate H ₃ (C)) + (12 (C)(O)) + (13 Literatur -677.50	-747.78 501.43 633.65 -1616.06 -265.95 107.28 c; Methyl penta 2 × C-(H) ₂ (C) ₂) 1 × O-(C)(CO)) ce - Calculated =	3.88 3.97 decylate + (1 × C-(H)	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂ O ₂ (CO)(C)) + Reference	Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ = \ln K_t =$ Ethyl ethan $(2 \times C - (H + L))$	H ₃ (C)) + (1 (H)(O)) Literatur se 144.35 hoate; Ethyl H ₃ (C)) + (1 (C)(O)), σ	- 421.85 154.80 248.85 - 365.13 - 312.99 126.26	1 = Residual - 10.45 C)) + (1 × O-(0	C)(CO)) + Reference 79FUC
$\Delta_t H^{\circ} = C_{\rho}^{\circ} = \frac{1}{C_{\rho}^{\circ}} = \frac{1}$	tadecanoate H ₃ (C)) + (12 (C)(O)) + (13 Literatur	364.30 -747.78 501.43 633.65 -1616.06 -265.95 107.28 c; Methyl penta 2 × C-(H) ₂ (C) ₂) 1 × O-(C)(CO)) c - Calculated = -680.03 387.19	3.88 3.97 decylate + (1 × C-(H)) = Residual	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂ O ₂ (CO)(C)) + Reference	Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ = \ln K_t =$ Ethyl ethan $(2 \times C - (H + L))$	H ₃ (C)) + (1 (H)(O)) Literatur se 144.35 hoate; Ethyl H ₃ (C)) + (1 (C)(O)), σ	- 421.85 154.80 248.85 - 365.13 - 312.99 126.26 acetate × C-(H) ₂ (O)(e	1 = Residual - 10.45 C)) + (1 × O-(0	C)(CO)) + Reference 79FUC C ₄ H ₈ O ₂ C)(CO)) +
$\Delta_t H^\circ = C_\rho^\circ = $ Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t = $ Methyl pen $(2 \times C - (I (1 \times CO - C_\rho^\circ = $	se -743.90 505.40 stadecanoate H ₃ (C)) + (12 (C)(O)) + (13 Literatur -677.50	-747.78 501.43 633.65 -1616.06 -265.95 107.28 c; Methyl penta 2 × C-(H) ₂ (C) ₂) 1 × O-(C)(CO)) c - Calculated = -680.03 387.19	3.88 3.97 decylate + (1 × C-(H)	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂ O ₂ (CO)(C)) + Reference	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ $\Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = $ $\ln K_{t} = $ Ethyl ethan $(2 \times C - (F_{t}) + C_{t})$	H ₃ (C)) + (1 (H)(O)) Literatur se 144.35 hoate; Ethyl H ₃ (C)) + (1 (C)(O)), σ	- 421.85 154.80 248.85 - 365.13 - 312.99 126.26 acetate × C-(H) ₂ (O)(e	1 = Residual - 10.45 C)) + (1 × O-(0	C)(CO)) + Reference 79FUC C4HeO2
$\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t =$ Methyl pen $(2 \times C - (I) \times CO - I)$ Gas phase $\Delta_t H^\circ = C_p^\circ = I$ Liquid pha $\Delta_t H^\circ = C_p^\circ = I$	tadecanoate H ₃ (C)) + (12 (C)(O)) + (13 Literatur	-747.78 501.43 633.65 -1616.06 -265.95 107.28 c; Methyl penta 2 × C-(H) ₂ (C) ₂) 1 × O-(C)(CO)) ce - Calculated = -680.03 387.19 -773.51 531.85	3.88 3.97 decylate + (1 × C-(H)) = Residual	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂ O ₂ (CO)(C)) + Reference	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = $ Liquid phas $\Delta_{t}H^{\circ} = S^{\circ} = $ $\Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = $ In $K_{t} = $ Ethyl ethan $(2 \times C - (f + 1) \times CO - f = 1)$ Gas phase	H ₃₃ (C)) + (1 (H)(O)) Literatur Se 144.35 noate; Ethyl H ₃ (C)) + (1 (C)(O), \(\sigma\)	- 388.42 86.86 - 421.85 154.80 248.85 - 365.13 - 312.99 126.26 acetate × C-(H) ₂ (O)(e = 9	1 = Residual - 10.45 C)) + (1 × O-(0) 1 = Residual	Reference 79FUC C ₄ H ₈ O ₂ C)(CO)) + Reference
$\Delta_t H^{\circ} = C_{\rho}^{\circ} = C_{\rho}^{\circ} = C_{\rho}^{\circ} = C_{\rho}^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = InK_t = C_{\rho}^{\circ} = InK_t = C_{\rho}^{\circ} = C_{\rho}^{\circ} = C_{\rho}^{\circ} = C_{\rho}^{\circ} = C_{\rho}^{\circ} = S^{\circ} = S^{\circ} = C_{\rho}^{\circ} = S^{\circ} = C_{\rho}^{\circ} = C_{\rho}^{\circ} = C_{\rho}^{\circ} = S^{\circ} = C_{\rho}^{\circ} = C_{\rho}^{\circ$	tadecanoate H ₃ (C)) + (12 (C)(O)) + (13 Literatur	-747.78 501.43 633.65 -1616.06 -265.95 107.28 2:; Methyl penta 2: C-(H) ₂ (C) ₂) 1: O-(C)(CO)) 2: - Calculated = -680.03 387.19 -773.51 531.85 666.03	3.88 3.97 decylate + (1 × C-(H)) = Residual	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂ O ₂ (CO)(C)) + Reference	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $\Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} =$ Ethyl ethan $(2 \times C - (I)(1 \times CO - I) = I)$ Gas phase $\Delta_{t}H^{\circ} = I$	H ₃₃ (C)) + (1 (H)(O)) Literatur See 144.35 Hoate; Ethyl H ₃ (C)) + (1 (C)(O)), \(\sigma\)	- 388.42 - 388.42 - 368.86 - 421.85 154.80 248.85 - 365.13 - 312.99 126.26 acetate × C-(H) ₂ (O)(e = 9	1 = Residual - 10.45 C)) + (1 × O-(0) 1 = Residual - 0.57	Reference 79FUC C4H8O2 C(CO)) + Reference
$\Delta_t H^\circ = C_p^\circ = \frac{1}{C_p^\circ} = \frac{1}{C_p^\circ$	tadecanoate H ₃ (C)) + (12 (C)(O)) + (13 Literatur	-747.78 501.43 633.65 -1616.06 -265.95 107.28 2: (Methyl pental 2: C-(H) ₂ (C) ₂) 1: O-(C)(CO)) 2: - Calculated = -680.03 387.19 -773.51 531.85 666.03 -1719.99	3.88 3.97 decylate + (1 × C-(H)) = Residual	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂ O ₂ (CO)(C)) + Reference	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $\Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} =$ Ethyl ethan $(2 \times C - (I + C) - I + C)$ Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$	H ₃ (C)) + (1 (H)(O)) Literatur Se 144.35 Hoate; Ethyl H ₃ (C)) + (1 (C)(O)), σ Literatur -444.10 113.64	~ C-(H) ₂ (O)(re - Calculated -388.42 86.86 -421.85 154.80 248.85 -365.13 -312.99 126.26 acetate × C-(H) ₂ (O)(e = 9	- 10.45 C)) + (1 × O-(0) 1 = Residual - 0.57 5.49	Reference 79FUC C4H ₈ O ₂ C)(CO))+ Reference 66WAD2 69STU/WES
$\Delta_t H^\circ = C_\rho^\circ = \frac{1}{C_\rho^\circ} = \frac{1}{C_\rho^\circ$	tadecanoate H ₃ (C)) + (12 (C)(O)) + (13 Literatur	-747.78 501.43 633.65 -1616.06 -265.95 107.28 2:; Methyl penta 2: C-(H) ₂ (C) ₂) 1: O-(C)(CO)) 2: - Calculated = -680.03 387.19 -773.51 531.85 666.03	3.88 3.97 decylate + (1 × C-(H)) = Residual	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂ O ₂ (CO)(C)) + Reference	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $\Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} =$ $\ln K_{t} =$ Ethyl ethan $(2 \times C - (f (1 \times CO - f)) = f (1 \times CO - f)$ Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = f (1 \times CO - f) = f (1 \times CO - f)$ $Gas phase$ $\Delta_{t}H^{\circ} = f (1 \times CO - f) = f (1 \times CO - f)$ $Gas phase$ $\Delta_{t}H^{\circ} = f (1 \times CO - f) = f (1 \times CO - f)$ $Gas phase$ $\Delta_{t}H^{\circ} = f (1 \times CO - f) = f (1 \times CO - f)$ $Gas phase$ $\Delta_{t}H^{\circ} = f (1 \times CO - f) = f (1 \times CO - f)$	H ₃₃ (C)) + (1 (H)(O)) Literatur See 144.35 Hoate; Ethyl H ₃ (C)) + (1 (C)(O)), \(\sigma\)	~ C-(H) ₂ (O)(re - Calculated -388.42 86.86 -421.85 154.80 248.85 -365.13 -312.99 126.26 acetate × C-(H) ₂ (O)(e = 9	1 = Residual - 10.45 C)) + (1 × O-(0) 1 = Residual - 0.57	Reference 79FUC C4H8O2 C(CO)) + Reference
$\Delta_t H^\circ = C_p^\circ = C_$	tadecanoate H ₃ (C)) + (12 (C)(O)) + (13 Literatur	-747.78 501.43 633.65 -1616.06 -265.95 107.28 2: (Methyl pental 2: C-(H) ₂ (C) ₂) 1: O-(C)(CO)) 2: - Calculated = -680.03 387.19 -773.51 531.85 666.03 -1719.99	3.88 3.97 decylate + (1 × C-(H)) = Residual	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂ O ₂ (CO)(C)) + Reference	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $\Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} =$ Ethyl ethan $(2 \times C - (I + C) - I + C)$ Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$	H ₃ (C)) + (1 (H)(O)) Literatur Se 144.35 Hoate; Ethyl H ₃ (C)) + (1 (C)(O)), σ Literatur -444.10 113.64	~ C-(H) ₂ (O)(re - Calculated -388.42 86.86 -421.85 154.80 248.85 -365.13 -312.99 126.26 acetate × C-(H) ₂ (O)(e = 9	- 10.45 C)) + (1 × O-(0) 1 = Residual - 0.57 5.49	Reference 79FUC C4H8O2 C)(CO))+ Reference 66WAD2 69STU/WES
$\Delta_t H^\circ = C_p^\circ = \frac{1}{C_p^\circ} = \frac{1}{C_p^\circ$	tadecanoate H ₃ (C)) + (12 (C)(O)) + (13 Literatur	-747.78 501.43 633.65 -1616.06 -265.95 107.28 c; Methyl penta 2 × C-(H) ₂ (C) ₂) 1 × O-(C)(CO)) e - Calculated = -680.03 387.19 -773.51 531.85 666.03 -1719.99 -260.70	3.88 3.97 decylate + (1 × C-(H)) = Residual	65ADR/DEK 79FUC C ₁₆ H ₃₂ O ₂ O ₂ (CO)(C)) + Reference	Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $\Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} =$ $\ln K_{f} =$ Ethyl ethan $(2 \times C - (f (1 \times CO - f)) = f (1 \times CO - f)$ Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = f (1 \times CO - f) = f (1 \times CO - f)$ $Gas phase$ $\Delta_{t}H^{\circ} = f (1 \times CO - f) = f (1 \times CO - f)$ $Gas phase$ $\Delta_{t}H^{\circ} = f (1 \times CO - f) = f (1 \times CO - f)$ $Gas phase$ $\Delta_{t}H^{\circ} = f (1 \times CO - f) = f (1 \times CO - f)$ $Gas phase$ $\Delta_{t}H^{\circ} = f (1 \times CO - f) = f (1 \times CO - f)$	H ₃ (C)) + (1 (H)(O)) Literatur Se 144.35 Hoate; Ethyl H ₃ (C)) + (1 (C)(O)), σ Literatur -444.10 113.64	~ C-(H) ₂ (O)(re - Calculated -388.42 86.86 -421.85 154.80 248.85 -365.13 -312.99 126.26 acetate × C-(H) ₂ (O)(e = 9	- 10.45 C)) + (1 × O-(0) 1 = Residual - 0.57 5.49	Reference 79FUC C4H8O2 C)(CO))+ Reference 66WAD2 69STU/WES

TADIE	21	Feters	(74)	_	Continued
IABLE	41.	Esters	(74)	_	Continued

Ethyl ethanoate; Ethyl acetate (Continued) $C_4H_8O_2$ $(2 \times C(H)_3(C)) + (1 \times C(H)_2(O)(C)) + (1 \times O(C)(CO)) + (1 \times CO(C)(O)), \sigma = 9$					2-Methylpropyl methanoate; Isobutyl formate $(2 \times C - (H)_3(C)) + (1 \times C - (H)(C)_3) + (1 \times C - (H)_2(O)(C)) + (1 \times O - (C)(CO)) + (1 \times CO - (H)(O)) + (2 \times - CH_3 \text{ corr (tertiary)})$				
	Literature	- Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
$C_p^{\circ} = S^{\circ} =$	478.80 169.20 259.41	-476.41 171.16 270.19	- 2.39 - 1.96 - 10.78	78FEN/HAR 33PAR/HUF 33PAR/HUF	Gas phase $\Delta_t H^\circ = C_\rho^\circ =$		-436.37 132.67		
$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	· · · · ·	-480.10 -333.27 134.44			Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = $	se 214.22	-478.59 212.66 308.26 -578.34	1.56	36KUR/VOS
	3(C))+(1)	yl acetate < C-(H) ₂ (C) ₂) × CO-(C)(O)		(O)(C) +	$\Delta_f G^\circ = \ln K_f =$		-306.16 123.50		
		e – Calculated		Reference	Butyl ethan				C ₆ H ₁₂ O ₂
Gas phase					(2×C-(H (1×O-(C	I)₃(C))+(2 C)(CO))+(\times C-(H) ₂ (C) ₂) 1 \times CO-(C)(O)	$+(1\times C-(H)_2)$	(O)(C))+
$\Delta_t H^\circ = C_p^\circ =$		-464.16 131.04					re – Calculated		Reference
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	196.07	-502.14 201.58 302.57	-5.51	86JIM/ROM	Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 485.60	-484.79 153.93	-0.81	66WAD2
$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$		-584.03 -328.01 132.32	none de la companya d		$C_p^{\circ} =$	e 529.20 228.45	- 527.87 232.00	-1.33 -3.55	58WAD 79FUC
(3×C-(H)) ₃ (C)) + (1:	opropyl acetat × C–(H)(O)(C . × CO–(C)(O))2 (ethers,este	$C_5H_{10}O_2$ rs)) + corr (tertiary))	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$		334.95 - 687.96 - 322.76 130.20		
, , , ,		e – Calculated		Reference	2.Methylpro	nyl ethano	ate; Isobutyl a	retate	C₅H ₁₂ O ₂
	- 481.70	-476.87	-4.83	66WAD2	(3×C-(H (1×C-(H	$(1)_3(C) + (1)_3(C)$	×CO-(C)(O)) +(1×C-(H)(C	+(1×O-(C)(CO))+
C _p =		131.33				Literatur	e – Calculated	= Residual	Reference
$C_p^{\circ} = S^{\circ} =$	-518.80 196.65	-513.58 199.56 295.59	- 5.22 - 2.91	58WAD 79FUC	Gas phase $\Delta_l H^\circ = C_p^\circ =$		-491.48 153.96		
$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = -$,	-591.01 -337.37 136.09			Liquid phas $\Delta_t H^o = C_r^o =$	e 240.20	-533.15 229.02	11.18	36KUR/VOS
					$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f = 0$		329.60 -693.31 -326.44 131.68		

TABLE 21. Esters (74) - Continued

(4×C-(H	(3)(C) + (1)	anoate; tert-But × C-(O)(C)3 (et l × CO-(C)(O))	hers,esters))	C ₆ H ₁₂ O ₂ + corr (quaternary))		$_{3}(C))+(3$	\times C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ ;)) + (1 × C-(H)	
	Literatur	e – Calculated =	Residual	Reference	***************************************	Literatur	e – Calculated	l = Residual	Reference
Gas phase					Gas phase				
$\Delta_i H^\circ = C_\rho^\circ =$		-499.33 153.88			$\Delta_t H^\circ = C_p^\circ =$		- 527.26 201.51		
Liquid phas $\Delta_t H^\circ =$	e	- 548.21			Liquid phase $\Delta_t H^\circ = -$	583.00	577 74	5.26	278.CU
$C_p^{\circ} =$	230.96	230.94	0.02	79FUC	$C_p^{\circ} =$	363.00	- 577.74 291.71	-5.26	37SCH
S° =	250.70	309.52	0.02	17100	$S^{\circ} =$		407.20		
$\Delta_t S^\circ =$		-713.39			$\Delta_f S^\circ =$		-888.33		
$\Delta_{\rm f}G^{\circ} =$		-335.51			$\Delta_{\rm f}G^{\circ} =$		-312.88		
$lnK_f =$		135.34			$lnK_f =$,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	126.22		
(2×C-(H	$I_{3}(C) + (1$	yl propionate ×C-(H) ₂ (O)(C 1×C-(H) ₂ (CO)		C ₅ H ₁₀ O ₂		3(C))+(4	\times C-(H) ₂ (C) ₂)) + (1 × C-(H) ₂ ()) + (1 × C-(H)	
	Literatur	re – Calculated =	- Residual	Reference		Literatur	e – Calculated	l = Residual	Reference
Gas phase	450.50		4.55		Gas phase		5.15.00		
$\Delta_t H^\circ = C_p^\circ =$	463.60	-465.37 132.84	1.77	72MAN2	$\Delta_{f}H^{\circ} = C_{p}^{\circ} =$		- 547.89 224.40		
Liquid phas					Liquid phase				
	-502.70	- 500.55	-2.15	72MAN2	•	613.30	-603.47	- 9.83	37SCH
$C_p^{\circ} =$	199.58	200.45	-0.87	87ZAB/HYN	$C_p^{\circ} =$		322.13		
S° =		310.06			S° =		439.58		
$\Delta_f S^\circ =$		-576.54			$\Delta_f S^\circ =$		- 992.26		
$\Delta_t G^\circ = \ln K_t =$		- 328.66 132.58			$\Delta_t G^\circ = \ln K_t =$		-307.63 124.09		
(2×C-(I	(C)(O))+(yi valerate 2 × C-(H) ₂ (C) ₂) - (1 × O-(C)(CO)) re – Calculated =	+ (1 × C-(H)			(C))+(1 corr (terti	\times C-(H) ₂ (C) ₂)	ı+(1×C-(H)(0 D-(C)(O))+(1	C ₆ H ₁₂ O ₂ CO)(C) ₂) + × O-(C)(CO)) +
						Literatur	e – Calculated	l = Residual	Reference
Gas phase $\Delta_t H^\circ =$		-506.63			Gas phase				
C _p =		178.62			•	492.50	-476.03	- 16.47	70COX/PIL
Liquid pha		552.01	0.00	2780U	Liquid phase	524 20	5 20.02	14 29	SALIA NAWA T
$\Delta_{\rm f}H^{\circ} =$	- 553.00	-552.01	-0.99	37SCH	-	534.30	- 520.02	14.28	54HAN/WAT
$C_p^{\circ} = S^{\circ} =$		261.29 374.82			$C_p^{\circ} = S^{\circ} =$		221.83 328.76		
$\Delta_{\rm f} S^{\circ} =$		374.82 784.40			$\Delta_t S^\circ =$		- 694.15		
$\Delta_{l}G^{\circ} =$		- 784.40 - 318.14			$\Delta_{f}S = \Delta_{f}G^{\circ} =$		- 094.13 - 313.06		
$lnK_f =$		128.34			$lnK_f =$		126.29		
urvt =		140.34			mar -		140.47		

TABLE 21. Esters (74) - Continued

(2×C-(I (1×C-(I	$\frac{1}{3}$ (C)) + (1 $\frac{1}{2}$ (CO)(C)	oate; Methyl iso × C-(H)(C) ₃) +) + (1 × CO-(C)	(2×-CH ₃ co		$(1 \times C_d - (1 \times C_d))$		nyl acetate d-(O)(H))+(1 ×C-(H) ₃ (C))	× O-(C _d)(CO)	C ₄ H ₆ O ₂
(1×C-(I	,	re – Calculated :	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase Δ _l H° =	- 497.90	- 480.42	-17.48	70COX/PIL	Gas phase Δ _t H° =	-314.90	- 314.89	-0.01	38DOL/GRE
$C_p^{\circ} =$ Liquid pha $\Delta_t H^{\circ} =$	se 538.90	158.32 - 521.49	- 17.41	54HAN/WAT	Liquid pha $\Delta_t H^\circ = C_p^\circ =$	- 349.70 165.40	- 345.60 154.01	-4.10 11.39	47STU 59BEN/THO
$C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = 0$		224.67 336.88 - 686.03 - 316.95 127.86			$(1 \times C_d -$	$(H)_2) + (1 \times$	ethyl acrylate C _d -(H)(CO)) + 1 × C-(H) ₃ (O)		C ₄ H ₆ O ₅ (O))+
-						Literatu	re – Calculated	= Residual	Reference
(3 × C-(H) ₃ (C))+(1 C)(CO))+(opanoate; Meth × C-(CO)(C) ₃) 3×-CH ₃ corr (re – Calculated	+(1×CO-(C quaternary))	$C_cH_{12}O_2$ C)(O)) + + (1 × C-(H) ₃ (O)) Reference	Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 333.00	- 309.24 99.08	-23.76	71HAL/BAL
Gas phase Δ _t H° =	-494.51	484.90	- 9.61	71HAL/BAL	Liquid pha $\Delta_t H^\circ = C_p^\circ =$	- 362.20 161.50	- 350.83 160.71	-11.37 0.79	71HAL/BAL 79FUC
Liquid pha $\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	se - 530.00 223.01	- 522.85 218.47 318.22 - 704.69 - 312.75 126.16	-7.15 4.54	71HAI /BAI. 71HAL/BAL	(1×C _d -($(H)_2) + (1 \times -(C_d)(O)) +$	noate; Methyl 1 C _d -(C)(CO)) + (1×O-(C)(CO culated = Resid	· (2×C−(H)₃(C	
Ethyl 2-me	ethylbutano	ate; Ethyl sec-v	ilerate	C ₇ H ₁₄ O ₂	Liquid pha $C_p^{\circ} =$	188.49	187.69	0.80	52ERD/JAG
(3×C-((1×CO	H) ₃ (C)) + (1 -(C)(O)) + (1 H ₃ corr (ter	$1 \times C - (H)_2(O)(C)$ $(1 \times C - (H)(CO))$	C))+(1×O-(((C) ₂)+(1×C	C)(CO))+	Methyl (2×C-(1	crotonate H)3(C))+(1	e; Methyl trans $\times O^{-}(C)(CO))$ $(1 \times C_{d^{-}}(H)(C)$	+(1×CO-(C ₆	C ₅ H ₈ O ₂
Gas phase $\Delta_t H^\circ =$	- 522.41	-508.93	- 13.48	70COX/PIL			re – Calculated	•	Reference
Liquid photon $\Delta_t H^\circ = C_\theta^\circ =$	nse - 566.81	-555.82 255.47	- 10.99	54HAN/WAT	Gas phase $\Delta_l H^\circ = C_p^\circ =$	- 341.92	-341.50 122.17	-0.42	70COX/PIL
$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$		361.35 - 797.87 - 317.94 128.25			Liquid pha $\Delta_f H^\circ = C_p^\circ =$	se 382.90	- 389.14 193.42	6.24	36SCH

TABLE 21. Esters (74) - Continued

Literature - Calculated = Residual

-387.84

-2.28

Gas phase $\Delta_t H^\circ = -390.12$

Reference

70COX/PIL

TABLE 21. Esters (/4) — Continued	TABLE 21. Esters (/4) — Continued
Ethyl (E)-2-butenoate; Ethyl trans-2-butenoate $(2 \times C - (H)_3(C)) + (1 \times C - (H)_2(O)(C)) + (1 \times C_d - (H)(C)) + (1 \times C_d - (H)(C)) + (1 \times C_d - (H)(C))$	Ethyl (Z)-2-pentenoate; Ethyl cis-2-pentenoate $(2 \times C - (H)_3(C)) + (1 \times C - (H)_2(O)(C)) + (1 \times O - (C)(CO)) + (1 \times CO - (C_d)(O)) + (1 \times C_d - (H)(CO)) + (1 \times C_d - (H)(C)) + (1 \times C - (H)_2(C)(C_d)) + (1 \times cis (unsat) corr)$
Literature - Calculated = Residual Reference	Literature - Calculated = Residual Reference
Gas phase $\Delta_l H^\circ = -375.60 -374.40 -1.20$ 70COX/PIL $C_p^\circ = 142.50$	Gas phase $\Delta_t H^\circ = -394.72 -390.43 -4.29$ 70COX/PIL $C_p^\circ = 155.10$
Liquid phase $\Delta_t H^\circ = -420.00 -424.94$ 4.94 36SCH $C_\rho^\circ =$ 227.06	Liquid phase $\Delta_t H^\circ = -440.80 -445.40$ 4.60 38SCH2 $C_p^\circ =$ 256.35
Ethyl-3-pentynoate $C_7H_{10}O_2$ $(2 \times C(H)_3(C)) + (1 \times C(H)_2(O)(C)) + (1 \times O(C)(CO)) + (1 \times CO(C)(O)) + (1 \times C(H)_2(CO)(C_1)) + (2 \times C_1-(C))$ Literature – Calculated = Residual Reference	$ \begin{array}{ll} \text{Ethyl (E)-2-pentenoate; Ethyl } \textit{trans-2-pentenoate} & C_7H_{12}O_2\\ (2\times C-(H)_3(C)) + (1\times C-(H)_2(O)(C)) + (1\times O-(C)(CO)) + \\ (1\times CO-(C_d)(O)) + (1\times C_d-(H)(CO)) + (1\times C_d-(H)(C)) + \\ (1\times C-(H)_2(C)(C_d)) \end{array} $
Gra whose	Literature – Calculated = Residual Reference
Gas phase $\Delta_t H^\circ = -237.82 -238.81$ 0.99 70COX/PIL	Gas phase
Liquid phase $\Delta_t H^\circ = -287.60 -288.72$ 1.12 38SCH	$\Delta_t H^\circ = -394.30 -395.28$ 0.98 70COX/PIL $C_p^\circ = 163.13$
Ethyl-4-pentynoate $C_7H_{10}O_2$ $(1 \times C - (H)_3(C)) + (1 \times C - (H)_2(O)(C)) + (1 \times O - (C)(CO)) + (1 \times C - (H)_2(C)(C)) + (1 \times C - (H)_2(C)(C)(C)) + (1 \times C - (H)_2(C)(C)(C)(C)) + (1 \times C - (H)_2(C)(C)(C)(C)(C)(C)(C)(C) + (1 \times C - (H)_2(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)($	Liquid phase $\Delta_t H^{\circ} = -442.50 - 450.67$ 8.17 38SCH2 $C_{\rho}^{\circ} = 256.35$
$(1 \times C_t - (C)) + (1 \times C_t - (H))$ Literature – Calculated = Residual Reference	Ethyl (Z)-3-pentenoate; Ethyl cis-3-pentenoate $C_7H_{12}O_2$ $(2 \times C-(H)_3(C)) + (1 \times C-(H)_2(O)(C)) + (1 \times O-(C)(CO)) + (1 \times CO-(C)(O)) + (1 \times C-(H)_2(CO)(C_d)) + (2 \times C_d-(H)(C)) +$
Gas phase $\Delta_t H^{\circ} = -233.22 -214.21 -19.01$ 70COX/PIL $C_p^{\circ} = 163.85$	$(1 \times cis \text{ (unsat) corr})$ Literature – Calculated = Residual Reference
Liquid phase $\Delta_t H^{\circ} = -281.71 - 263.45 - 18.26$ 38SCH	Gas phase $\Delta_t H^\circ = -387.61 - 382.99 - 4.62$ 70COX/PIL
$C_p^{\circ} = 259.91$ $S^{\circ} = 340.94$ $\Delta_t S^{\circ} = -557.14$ $\Delta_t G^{\circ} = -97.34$ $\ln K_t = 39.27$	Liquid phase $\Delta_t H^\circ = -432.40 - 428.66 - 3.74$ 38SCH2
	Ethyl (E)-3-pentenoate; Ethyl trans-3-pentenoate $C_7H_{12}O_2$ $(2 \times C-(H)_3(C)) + (1 \times C-(H)_2(O)(C)) + (1 \times O-(C)(CO)) + (1 \times CO-(C)(O)) + (1 \times C-(H)_2(CO)(C_d)) + (2 \times C_d-(H)(C))$

 $C_7H_{12}O_2$

TABLE 21. Esters (74) - Continued

TABLE 21. Esters (74) - Continued

Ethyl (E)-3-pentenoate; Ethyl trans-3-pentenoate (Continued) C7H12O2
$(2 \times C - (H)_3(C)) + (1 \times C - (H)_2(O)(C)) + (1 \times O - (C)(CO)) +$
$(1 \times CO - (C)(O)) + (1 \times C - (H)_2(CO)(C_d)) + (2 \times C_d - (H)(C))$

	Literature – Calculated = Residual				
Liquid ph $\Delta_t H^\circ =$	ase -437.00	-433.93	-3.07	38SCH2	

$\begin{array}{ll} \textbf{Propyl (E)-2-butenoate; Propyl } \textit{trans-2-butenoate} & \textbf{C}_{7}\textbf{H}_{12}\textbf{O}_{2} \\ & (2\times C-(H)_{3}(C))+(1\times C-(H)_{2}(C)_{2})+(1\times C-(H)_{2}(O)(C))+\\ & (1\times O-(C)(CO))+(1\times CO-(C_{d})(O))+(1\times C_{d}-(H)(CO))+\\ & (1\times C_{d}-(H)(C)) \end{array}$

	Literature - Calculated = Residual					
Liquid ph $\Delta_{f}H^{\circ} = C_{p}^{\circ} =$	nase 443.30	- 450.67 257.48	7.37	36SCH		

$\begin{array}{ll} \textbf{Ethyl 4-pentenoate} & & & & & & \\ (1\times C-(H)_3(C))+(1\times C-(H)_2(O)(C))+(1\times O-(C)(CO))+\\ (1\times CO-(C)(O))+(1\times C-(H)_2(CO)(C))+(1\times C-(H)_2(C)(C_d))+\\ (1\times C_d-(H)(C))+(1\times C_d-(H)_2) \end{array}$

	Literature – Calculated = Residual			Reference	
Gas phase					
$\Delta_f H^\circ =$	- 385.51	- 381.35	-4.16	70COX/PIL	
$C_p^{\circ} =$		167.86			
Liquid ph	ase				
	ase -431.60	-425.87 246.23	-5.73	37SCH	
$\Delta_l H^\circ = C_p^\circ =$		246.23	-5.73	37SCH	
$\Delta_t H^\circ = C_p^\circ = S^\circ = S$		246.23 373.20	-5.73	37SCH	
$\Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} =$		246.23 373.20 - 655.45	-5.73	37SCH	
$\Delta_t H^\circ = C_p^\circ = S^\circ = S$		246.23 373.20	-5.73	378СН	

Isopropyl (E)-2-butenoate; Isopropyl trans-2-butenoate

$(3 \times C - (H)_3(C)) + (1 \times C_d - (H)(C)) + (1 \times C_d - (H)(CO)) +$
$(1 \times CO - (C_d)(O)) + (1 \times O - (C)(CO)) +$
$(1 \times C - (H)(O)(C)_2$ (ethers, esters)) +
(2×-CH ₃ corr (tertiary))

	Literature – Calculated = Residual				
Gas phase $\Delta_t H^\circ = -C_p^\circ =$	411.10	- 407.74 165.68	- 3.36	70COX/PIL	
Liquid phase $\Delta_l H^\circ = -C_p^\circ =$		-462.11 255.46	5.01	36SCH	

$\begin{array}{c} \textbf{Ethyl-2,4-pentadienoate} & C_7H_{10}O_2\\ (1\times C-(H)_3(C)) + (1\times C-(H)_2(O)(C)) + (1\times O-(C)(CO)) + \end{array}$

 $(1 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)(C)) + (1 \times C - (H)(C_d)) + (1 \times C_d - (H)(C_d)) + (1 \times C_d - (H)_2)$

L	Reference		
Gas phase $\Delta_t H^\circ = -2t$ $C_p^\circ =$	89.70 — 286.09 156.49	-3.61	70COX/PIL
Liquid phase $\Delta_t H^\circ = -33$ $C_p^\circ =$	38.20 - 336.08 254.51	-2.12	38SCH

$\begin{array}{ll} \text{Butyl (E)-2-butenoate; Butyl } \textit{trans-2-butenoate} & C_8H_{14}O_2\\ (2\times C-(H)_3(C))+(2\times C-(H)_2(C)_2)+(1\times C-(H)_2(O)(C))+\\ (1\times O-(C)(CO))+(1\times CO-(C_d)(O))+(1\times C_d-(H)(CO))+\\ (1\times C_d-(H)(C)) & \end{array}$

Literatu	Reference		
Gas phase $\Delta_t H^\circ = -415.89$ $C_p^\circ =$	-415.66 188.28	- 0.23	70COX/PIL
Liquid phase $\Delta_t H^\circ = -467.80$ $C_\rho^\circ =$	- 476.40 287.90	8.60	36SCH

$\begin{array}{ll} \textbf{Propyl (E)-2-butenoate; Propyl trans-2-butenoate} & C_7H_{12}O_2\\ (2\times C-(H)_3(C))+(1\times C-(H)_2(C)_2)+(1\times C-(H)_2(O)(C))+\\ (1\times O-(C)(CO))+(1\times CO-(C_d)(O))+(1\times C_d-(H)(CO))+\\ (1\times C_d-(H)(C)) & \end{array}$

	Literatur	Reference		
Gas phase $\Delta_t H^\circ = C_p^\circ =$		- 395.03 165.39	0.73	70COX/PIL

$\begin{array}{ll} \textbf{Propyl 2-pentenoate} & \textbf{C}_{\textbf{g}}\textbf{H}_{\textbf{14}}\textbf{O}_{\textbf{2}} \\ & (2 \times \textbf{C} - (\textbf{H})_3(\textbf{C})) + (1 \times \textbf{C} - (\textbf{H})_2(\textbf{C})_2) + (1 \times \textbf{C} - (\textbf{H})_2(\textbf{O})(\textbf{C})) + \\ & (1 \times \textbf{O} - (\textbf{C})(\textbf{CO})) + (1 \times \textbf{CO} - (\textbf{C}_{\textbf{d}})(\textbf{O})) + (1 \times \textbf{C}_{\textbf{d}} - (\textbf{H})(\textbf{CO})) + \\ & (1 \times \textbf{C}_{\textbf{d}} - (\textbf{H})(\textbf{C})) + (1 \times \textbf{C} - (\textbf{H})_2(\textbf{C})(\textbf{C}_{\textbf{d}})) \end{array}$

	Literatui	Reference		
Gas phase $\Delta_t H^\circ = C_p^\circ =$	-413.00	-415.91 186.02	2.91	70COX/PIL

 $C_8H_{14}O_2$

C₈H₁₄O₂

Reference

37SCH

Reference

70COX/PIL

 $C_8H_{14}O_2$

37SCH

Liquid phase $\Delta_f H^\circ = -$

 $C_p^{\circ} =$

Gas phase $\Delta_f H^\circ = -404.22$

Liquid phase $\Delta_f H^{\circ} = -454.40$

Isopropyl 3-pentenoate

 $(1 \times C - (H)_2(C)(C_d))$

Propyl 3-pentenoate

 $(2 \times C_{d}-(H)(C))$

Propyl 2-pentenoate (Continued)

-464.90

 $(1 \times C_a - (H)(C)) + (1 \times C - (H)_2(C)(C_a))$

TABLE	21	Ecters	(74)	Continued
I ABLE	21.	CSICIS	(/4) -	Continued

 $(2 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(O)(C)) + (1 \times O - (C)(CO)) + (1 \times CO - (C_d)(O)) + (1 \times C_d - (H)(CO)) + (1 \times C_d - (H)(CO))$

Literature - Calculated = Residual

-476.40

286.77

 $\begin{array}{l} (2 \times C - (H)_2(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(O)(C)) + \\ (1 \times O - (C)(CO)) + (1 \times CO - (C)(O)) + (1 \times C - (H)_2(CO)(C_d)) + \\ \end{array}$

Literature - Calculated - Residual

-408.47

-459.66

 $(2 \times C_d - (H)(C)) + (2 \times -CH_3 \text{ corr (tertiary)}) +$

11.50

4.25

5.26

Literatur	e – Calculated		
		= Residual	Reference
	-671.12 155.40		
	745.16		
263.17	264.68	- 1.51	30WAS
,(C)) + (2: 0)(CO))	× C-(H) ₂ (O)(C		C_6H_{10} $C)(CO)) +$ Reference
742.00	- 775.56	33.56	47STU
18-T			
805.50 260.66	-805.46 260.66	- 0.04 0.00	66ZIM/ROB 1881REI
(C))+(2		+(2×CO-(C)	C ₇ H ₁₂ (O))+
141			
. , , ,	e – Calculated	= Residual	Reference
. , , ,		– Residual	Reference
. , , ,	v — Calculated	- Residual	Reference
. , , ,	- 833.26	Residual	
284.93 edioate; D	- 833.26	0.01 le ())+(2×O-(C	33KOL/UDO C ₈ H ₁₄
284.93 edioate; D (C)) + (2)	- 833.26 - 880.65 284.92 Diethyl succinal	0.01 te (2) + (2 × O-(C) (C))	33KOL/UDC
284.93 edioate; D (C)) + (2)	- 833.26 - 880.65 284.92 biethyl succinal < C-(H) ₂ (O)(C	0.01 te (2) + (2 × O-(C) (C))	33KOL/UDO C ₈ H ₁₄ (C)(CO)) +
	742.00 805.50 260.66	nedioate; Diethyl oxalate $S(C) + (2 \times C - (H)_2(O)(C))$ $S(C) + (2 \times C - (H)_2(O)(C))$ Literature – Calculated $S(C) + (2 \times C - (H)_2(O)(C)$ $S(C) + (2 \times C - (H)_2(O)(C)(C)$ $S(C) + (2 \times C - (H)_2(O)(C)(C)$ $S(C) + (2 \times C - (H)_2(O)(C)(C)(C)$ $S(C) + (2 \times C - (H)_2(O)(C)(C)(C)$ $S(C) + (2 \times C - (H)_2(O)(C)(C)(C)$ $S(C) + (2 \times C - (H)_2(O)(C)(C)(C)(C)$ $S(C) + (2 \times C - (H)_2(O)(C)(C)(C)(C)(C)$ $S(C) + (2 \times C - (H)_2(O)(C)(C)(C)(C)(C)$	263.17 264.68 -1.51 redioate; Diethyl oxalate $s(C) + (2 \times C - (H)_2(O)(C)) + (2 \times O - (C))(CO)$ Literature - Calculated = Residual 742.00 -775.56 33.56

	Literature - Calculated = Residual			Reference	
Gas phase Δ _t H° =	- 425.09	- 442.06	16.97	70COX/PIL	
Liquid pha Δ _ε H° =		-496.83	23.53	37SCH	
	H) ₃ (C))+(2	; Dimethyl oxa × O-(C)(CO))	+(2×CO-(O		
	Literatui	re – Calculated	= Residuai	Reference	
Gas phase $\Delta_t H^\circ =$	- 708.90	709.76	0.86	76ANT/CAR	
Liquid ph	ase -735.20		-1.34	76ANT/CAR	
$C_p^{\circ} =$		193.38			

TABLE 21. Esters (74) - Continued

Diethyl butanedioate; Diethyl succinate (Continued) C₈H₁₄O₄ $(2 \times C - (H)_3(C)) + (2 \times C - (H)_2(O)(C)) + (2 \times O - (C)(CO)) +$

 $(2 \times CO - (C)(O)) + (2 \times C - (H)_2(CO)(C))$

	Literatu	re – Calculated =	Reference	
Liquid pha	se	·		
$\Delta_t H^{\circ} =$		- 905.88		
$C_p^{\circ} =$	330.54	327.94	2.60	79FUC
$C_p^{\circ} = S^{\circ} =$		453.52		
$\Delta_t S^\circ =$		- 916.48		
$\Delta_t G^{\circ} =$		-632.63		
$lnK_f =$		255.20		
-				

2-Oxetanone; 3-Propanolactone; β-Propiolactone

C₃H₄O₂ $(1 \times C - (H)_2(CO)(C)) + (1 \times C - (H)_2(O)(C)) + (1 \times O - (C)(CO)) +$ $(1 \times CO-(C)(O)) + (1 \times \beta$ -propiolactone rsc)

Literature - Calculated = Residual Reference Gas phase 0.00 66BOR/NAK $\Delta_{f}H^{\circ} =$ -282.90-282.90Liquid phase $\Delta_f H^\circ =$ -329.90-329.900.00 66BOR/NAK $C_p^{\circ} = S^{\circ} =$ 0.00 83LEB/YEV 122.09 122.09 175.31 175.31 0.00 83LEB/YEV $\Delta_{\epsilon}S^{\circ} =$ -308.10 $\Delta_f G^\circ =$ -238.04 $lnK_f =$ 96.02

4-Butanolactone; τ-Butyrolactone

C₄H₆O₂ $(1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) + (1 \times C - (H)_2(O)(C)) +$ $(1 \times O - (C)(CO)) + (1 \times CO - (C)(O)) + (1 \times \tau$ -butyrolactone rsc)

	Literatu	Reference		
Gas phase $\Delta_t H^\circ =$	- 366.50	-366.50	0.00	90LEI/PIL
Liquid ph	ase			
$\Delta_t H^{\circ} =$	-420.90	-420.90	0.00	90LEI/PIL
$C_p^{\circ} =$	141.29	141.30	-0.01	83LEB/YEV
s° =	197.40	197.40	0.00	83LEB/YEV
$\Delta_f S^\circ =$		-422.32		
$\Delta_f G^\circ =$		- 294.99		
$lnK_f =$		119.00		

4-Pentanolactone; τ-Valerolactone

C₅H₈O₂

 $(1 \times C - (H)_2(C)_2) + (1 \times C - (H)(O)(C)_2 \text{ (ethers, esters)}) +$

 $(1 \times C - (H)_3(C)) + (1 \times - CH_3 \text{ corr (tertiary)}) +$

 $(1 \times C - (H)_2(CO)(C)) + (1 \times O - (C)(CO)) + (1 \times CO - (C)(O)) +$

(1×τ-Valerolactone rsc)

Literatur	Reference		
Gas phase $\Delta_t H^{\circ} = -406.50$	- 406.50	0.00	90LEI/PIL
Liquid phase $\Delta_t H^\circ = -461.30$	- 461.30	0.00	90LEI/PIL

5-Pentanolactone; δ-Valerolactone

C5H8O2

 $(2 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) + (1 \times C - (H)_2(O)(C)) +$ $(1 \times O - (C)(CO)) + (1 \times CO - (C)(O)) + (1 \times \delta$ -valerolactone rsc)

	Literatur	re – Calculated =	= Residual	Reference		
Gas phase	Gas phase					
$\Delta_f H^\circ =$	- 379.60	- 379.60 	0.00	90LEI/PIL		
Liquid ph	iase					
$\Delta_t H^\circ =$	-437.60	-437.60	0.00	90LEI/PIL		
$C_{r}^{\circ} =$	171.59	171.59	0.00	83LEB/YEV		
S° =	218.99	218.99	0.00	83LEB/YEV		
$\Delta_f S^\circ =$		- 537.04		,		
$\Delta_t G^{\circ} =$		- 277.48				
$\ln K_t =$		111.93				

Hexanolactone; Caprolactone

 $C_6H_{10}O_2$

 $(3 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) + (1 \times C - (H)_2(O)(C)) +$ $(1 \times O - (C)(CO)) + (1 \times CO - (C)(O)) + (1 \times caprolactone rsc)$

	Litera	Literature-Calculated = Residual			
Liquid pha	ise				
$C_p^{\circ} =$	196.82	196.83	-0.01	83LEB/YEV	
S° =	235.68	235.68	0.00	83LEB/YEV	
$\Delta_t S^\circ =$		- 656.66			

Undecanolactone

 $C_{11}H_{20}O_2$

 $(8 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) + (1 \times C - (H)_2(O)(C)) +$ $(1 \times O - (C)(CO)) + (1 \times CO - (C)(O)) + (1 \times undecanolactone rsc)$

	Literature-Calculated = Residual			Reference	
Liquid pha	se				
$C_p^{\circ} =$	342.71	342.73	-0.02	83LEB/YEV	
S° =	369.49	369.45	0.04	83LEB/YEV	
$\Delta s^{\circ} =$		- 1204.44			

TABLE	21	Ectore	(74)	- Continued
LABLE	Z1.	ESIEIS	(/4) -	- Conunuea

	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	l = Residual	Reference
· · · · · · · · · · · · · · · · · · ·					Gos phase				
Gas phase $\Delta_t H^\circ =$	-287.90	-271.58	- 16.32	71KUS/WAD	Gas phase $\Delta_t H^\circ = -$	- 142.60	- 143.15	0.55	71CAR/FIN
$\begin{array}{l} \text{Liquid phas} \\ \Delta_t H^\circ = \\ C_p^\circ = \end{array}$	se -343.50	-332.33 222.01	- 11.17	71HAL/BAL	Liquid phase $\Delta_t H^\circ =$	e	- 219.01		
henyl eth:	anoate; Phei	nyl acetate		C ₈ H ₈ O ₂	Solid phase $\Delta_t H^\circ = C_0^\circ =$	- 241.60	- 240.55 230.95	-1.05	67ADA/FIN
(1×C-(I	$H_{3}(C) + (1$	\times CO-(C)(O)) (5 \times C _B -(H)(C			$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ}$		306.62 - 625.90 - 53.94		
	Literatur	e – Calculated	= Residual	Reference	$lnK_f =$		21.76		
Gas phase $\Delta_t H^\circ =$	-279.70	- 282.20	2.50	72LEB/KAT	Dimethyl 1,2 Dimethyl		; Dimethyl o-p	ohthalate;	C10H10
					(2 x C-(H	(C) + (2	×O-(C)(CO))	+(2×CO-(C	$O(C_{\rm B})) +$
$\Delta_t H^\circ = \frac{1}{2}$ Ethyl benze $(1 \times C - (1)$	-325.40 oate H) ₃ (C))+(1	- 327.29 × C-(H) ₂ (O)((1 × C _B -(CO))			$(2 \times C_B - (C_B - C_B))$ Gas phase $\Delta_t H^o =$	CO)(C _B) ₂) -	+ (4 × C _B -(H)(ce - Calculated		Reference
$\Delta_t H^\circ =$ Ethyl benze $(1 \times C - (1 \times C))$	-325.40 oate H) ₃ (C)) + (1 -(O)(C _B)) + (C)) + (1 × O-(0 C _B) ₂) + (5 × C _E	C ₉ H ₁₀ O ₂	(2×C _B -(C	CO)(C _B) ₂) -	e – Calculated		
$\Delta_t H^\circ =$ Ethyl benze $(1 \times C - (1 \times CO - 1))$	-325.40 oate H) ₃ (C)) + (1 -(O)(C _B)) + (×C-(H) ₂ (O)(((1×C _B -(CO)(C)) + (1 × O-(0 C _B) ₂) + (5 × C _E	C ₉ H ₁₀ O ₂ C)(CO)) + (H)(C _B) ₂)	$(2 \times C_B - (C_B - (C_$	CO)(C _B) ₂) -	e – Calculated – 624.76		
Ethyl benz (1×C-(I (1×CO-	-325.40 oate H) ₃ (C)) + (1 -(O)(C _B)) + (× C-(H) ₂ (O)(((1 × C _B -(CO)(re – Calculated	C)) + (1 × O-(0 C _B) ₂) + (5 × C _E	C ₉ H ₁₀ O ₂ C)(CO)) + (H)(C _B) ₂)	$(2 \times C_B - (C_B - C_B))$ Gas phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ Dimethyl 1,3 Dimethyl (2 \times C - (H)	ECO)(C _B) ₂) - Literatur e 309.28 3-phthalate isophthala) ₃ (C)) + (2	- 624.76 - 710.36 311.44 ; Dimethyl m-	= Residual -2.16 phthalate; +(2×CO-(C)	Reference 78MIL C ₁₀ H ₁₀ (0)(C _B))+
$\Delta_t H^\circ =$ Ethyl benza $(1 \times C - (1 \times C) - (1 \times C)$ Gas phase $\Delta_t H^\circ =$ Liquid pha $\Delta_t H^\circ =$	-325.40 oate H) ₃ (C)) + (1 -(O)(C _B)) + (Literatur	\times C-(H) ₂ (O)((1 \times C _B -(CO)() re - Calculated - 304.48	$C(T) + (1 \times O - (0 \times O)) + (5 \times C_E)$ $C(T) = Residual$	C ₉ H ₁₀ O ₂ C)(CO)) + -(H)(C _B) ₂) Reference	$(2 \times C_B - (C_B - C_B))$ Gas phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ Dimethyl 1,3 Dimethyl (2 \times C - (H)	Literatur 309.28 -phthalate isophthala)3(C)) + (2 CO)(C _B) ₂) +	- 624.76 - 710.36 311.44 ; Dimethyl m-te × O-(C)(CO))	= Residual -2.16 phthalate; +(2 × CO-(CC _B) ₂) + (1 × max	78MIL C ₁₀ H ₁₀ (C ₈))+
Ethyl benzz $(1 \times C - (1 \times C) - (1 \times C)$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p^\circ = C_p^\circ = C_p^\circ$	-325.40 oate H) ₃ (C)) + (1 -(O)(C _B)) + (1 Literatur ase 246.00 henyl ethano H) ₃ (C)) + (1 (O)(C _B) ₂) + (1	\times C-(H) ₂ (O)((1 \times C _B -(CO)() re - Calculated - 304.48	C)) + (1 × O-(0 C _B) ₂) + (5 × C _E = Residual -9.65 chenyl acetate + (1 × O-(C _B)	C ₉ H ₁₀ O ₂ C)(CO)) + r(H)(C _B) ₂) Reference 79FUC C ₉ H ₁₀ O ₂	$(2 \times C_B - (C_B - C_B))$ Gas phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ Dimethyl 1,3 Dimethyl (2 \times C - (H)	Literatur 309.28 -phthalate isophthala)3(C)) + (2 CO)(C _B) ₂) +	- 624.76 - 710.36 311.44 ; Dimethyl m-te ×O-(C)(CO)) + (4×C _B -(H)(6)	= Residual -2.16 phthalate; +(2 × CO-(CC _B) ₂) + (1 × max	Reference 78MIL C ₁₀ H ₁₀ (0)(C _B)) + eta corr)
Ethyl benzz $(1 \times C - (1 \times C) - (1 \times C)$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p^\circ = C_p^\circ = C_p^\circ$	-325.40 oate H) ₃ (C)) + (1 -(O)(C _B)) + (1 Literatur ase 246.00 henyl ethano H) ₃ (C)) + (1 (O)(C _B) ₂) + (2 c corr)	× C-(H) ₂ (O)((1 × C _B -(CO)((1 × C _B -(CO)((1 × C _B -(CO)((1 × C _B -(CO)((1 × CO)((1 × CO)((C)) + (1 × O-(0 C_{B})2) + (5 × C_{E}) = Residual -9.65 Chenyl acetate + (1 × O-(C_{B}) B)2) + (1 × C_{B} -1	C ₉ H ₁₀ O ₂ C)(CO)) + r(H)(C _B) ₂) Reference 79FUC C ₉ H ₁₀ O ₂	Gas phase $\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_p^\circ =$ Dimethyl 1,3 Dimethyl (2 × C-(H) (2 × C _B -(C)	ECO)(C _B) ₂) - Literatur 309.28 3-phthalate isophthala) ₃ (C)) + (2 CO)(C _B) ₂) + Literatur	- 624.76 - 710.36 311.44 ; Dimethyl m- te × O-(C)(CO)) + (4 × C _B -(H)(0) e - Calculated	= Residual -2.16 phthalate; +(2 × CO-(CC _B) ₂) + (1 × max	Reference 78MIL C ₁₀ H ₁₀ (0)(C _B)) + eta corr)

TABLE 21. Esters (74) - Continued

Dimethyl 1,3-phthalate; Dimethyl m-phthalate;

Dimethyl isophthalate (Continued)

 $C_{10}H_{10}O_4$

 $\begin{array}{l} (2\times C-(H)_3(C)) + (2\times O-(C)(CO)) + (2\times CO-(O)(C_B)) + \\ (2\times C_B-(CO)(C_B)_2) + (4\times C_B-(H)(C_B)_2) + (1\times \textit{meta} \ \textit{corr}) \end{array}$

Literatu	Literature - Calculated = Residual		
Solid phase			
$\Delta_t H^{\circ} = -730.90$	-760.26	29.36	72COL/LAY
$C_p^{\circ} =$	205.14		
S° =	292.98		
$\Delta_{\mathbf{f}}S^{\circ} =$	-827.36		
$\Delta_{\rm f}G^{\circ} =$	-513.58		
$lnK_f =$	207.18		

Dimethyl 1,4-phthalate; Dimethyl p-phthalate;

Dimethyl terephthalate

CtoHtoO4

 $(2 \times C - (H)_3(C)) + (2 \times O - (C)(CO)) + (2 \times C_B - (CO)(C_B)_2) + (4 \times C_B - (H)(C_B)_2) + (2 \times CO - (O)(C_B))$

	Literatur	Reference			
Gas phase					
Δ ₁ H° -		- 626.02 			
Liquid pha	ase				
$\Delta_{i}H^{\circ}$ -		-713.62			
C _p =		307.94			
Solid phas	se				
$\Delta_{\rm f} H^{\circ} =$	-732.60	-762.26	29.66	72COL/LAY	
$C_p^{\circ} =$	261.08	205.14	55.94	68ELL/CHR	
S° =		292.98			
Δ _f S° -		827.36			
$\Delta_r G^\circ =$		-515.58			
$lnK_{f} =$		207.98			

Diethyl 1,2-phthalate; Diethyl o-phthalate;

Diethyl phthalate

 $C_{12}H_{14}O_4$

 $\begin{array}{l} (2\times C-(H)_3(C)) + (2\times C-(H)_2(O)(C)) + (2\times O-(C)(CO)) + \\ (2\times CO-(O)(C_B)) + (2\times C_B-(CO)(C_B)_2) + (4\times C_B-(H)(C_B)_2) + \\ (1\times ortho\ corr) \end{array}$

Literat	Literature — Calculated — Residual				
Gas phase $\Delta_t H^\circ = -688.40$	- 690.56	2.16	58НОҮ/РЕР		
Liquid phase $\Delta_t H^\circ = -776.60$ $C_\rho^\circ = 366.15$	- 781.96 378.72	5.36 12.57	52MED/THO 67CHA/HOR		

Cyclobutane methyl carboxylate

C₆H₁₆O₂

 $(3 \times C - (H)_2(C)_2) + (1 \times C - (H)(CO)(C)_2) + (1 \times CO - (C)(O)) + (1 \times O - (C)(CO)) + (1 \times C - (H)_3(O)) +$

(1×Cyclobutane methyl carboxylate rsc)

Literatu	Literature – Calculated = Residual				
Gas phase $\Delta_t H^\circ = -355.30$	- 355.30	0.00	71HAL/BAL		
Liquid phase $\Delta_t H^{\circ} = -395.00$	- 395.00	0.00	71HAL/BAL		

Bicyclobutane methyl carboxylate

C₆H₈O₂

 $(2 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)_3) + (1 \times C - (CO)(C)_3) + (1 \times CO - (C)(O)) + (1 \times O - (C)(CO)) + (1 \times C - (H)_2(O)) + (1 \times C$

(1 × Bicyclobutane methyl carboxylate rsc)

Literatu	Literature – Calculated = Residual		
Gas phase $\Delta_t H^\circ = -164.60$	- 164.60	0.00	71HAL/BAL
Liquid phase $\Delta_t H^\circ = -203.10$	-203.10	0.00	71HAL/BAL

Cubane 1,4-dimethyldicarboxylate

 $C_{12}H_{12}O_4$

 $(6 \times C - (H)(C)_3) + (2 \times C - (CO)(C)_3) + (2 \times CO - (C)(O)) + (2 \times O - (C)(CO)) + (2 \times C - (H)_3(O)) +$

(1×1,4-Dimethylcubane dicarboxylate)

Literatu	Literature – Calculated – Residual				
Gas phase Δ _f H° 100.10	- 100.10	0.00	66KYB/CAR		
Solid phase $\Delta_t H^\circ = -218.99$	- 218.99	0.00	89KIR/CHU		

Solid phase $\Delta_t H^\circ = -369.60 -369.40$

-0.20

75CAR/LAY

TABLE 22. Peroxides (7)		TABLE 22. Peroxides (7) - Continue	ed	
Dimethylperoxide $(2 \times C-(H)_3(C)) + (2 \times O-(C)(O))$	C₂H₅O₂	Diacetyl peroxide; Diethanoyl peroxide $(2 \times C - (H)_3(CO)) + (2 \times CO - (C)(O)) + (2 \times O - (CO)(C)(O))$		
Literature – Calculated = Residual	Reference	Literature - Calculated = Residual	Reference	
Gas phase $\Delta_t H^\circ = v - 125.90 - 126.02$ 0.12	65BAK/LIT	Gas phase $\Delta_t H^{\circ} = -535.00$		
Diethylperoxide (2×C-(H) ₃ (C)) + (2×C-(H) ₂ (O)(C)) + (2×O-(C	C ₄ H ₁₀ O ₂	Liquid phase $\Delta_t H^\circ = -535.30 -573.96$ 38.66	57JAF/PRO	
Literature – Calculated = Residual	Reference	Dipropionyl peroxide; Dipropanoyl peroxide	C ₆ H ₁₀ O ₄	
Gas phase $\Delta_t H^\circ = -192.80 -191.82 -0.98$	39BLA/GER	$(2 \times C - (H)_3(C)) + (2 \times C - (H)_2(CO)(C)) + (2 \times CO - (2 \times O - (CO)(O)))$		
· · · · · · · · · · · · · · · · · · ·		Literature – Calculated = Residual	Reference	
Liquid phase $\Delta_t H^\circ = -223.30 -213.82 -9.48$	65BAK/LIT	Gas phase $\Delta_t H^{\circ} = -578.68$		
Di-tert-butyl peroxide $(6 \times C-(H)_3(C)) + (2 \times O-(C)(O)) +$ $(2 \times C-(O)(C)_3$ (alcohols,peroxides)) + $(6 \times -CH_3 \text{ corr (quaternary)})$	C ₈ H ₁₈ O ₂	Liquid phase $\Delta_f H^o = -620.10 -622.24$ 2.14	57JAF/PRO	
Literature – Calculated = Residual	Reference	Dibutyryl peroxide; Dibutanoyl peroxide (2×C-(H) ₃ (C))+(4×C-(H) ₂ (CO)(C))+(2×CO-((2×O-(CO)(O))	C ₈ H ₁₄ O ₄ (C)(O))+	
Gas phase $\Delta_t H^{\circ} = -349.11 -349.42$ 0.31	51EGE/EMT	Literature – Calculated = Residual	Reference	
Liquid phase $\Delta_t H^{\circ} = -380.91 -381.26$ 0.35	65BAK/LIT	Gas phase $\Delta_t H^\circ = -622.36$		
Dibenzoyl peroxide $(10\times C_B-(H)(C_B)_2)+(2\times C_B-(CO)(C_B)_2)+(2\times C_B)$ $(2\times O-(CO)(O))$	$C_{14}H_{10}O_4$ CO-(O)(C _B)) +	Liquid phase $\Delta_t H^\circ = -673.60 -670.52 -3.08$	57JAF/PRO	
Literature - Calculated = Residual	Reference			
Gas phase $\Delta_t H^{\circ} = -271.70 -256.90 -14.80$	75CAR/LAY			
Liquid phase $\Delta_t H^{\circ} = -357.40$	-			

TABLE	23.	Hydroperoxides ((9)	

TABLE 23. Hydroperoxides (9) - Continued

tert-Butyl hydroperoxide $C_4H_{10}O_2$ $(3 \times C-(H)_3(C)) + (1 \times C-(O)(C)_3 \text{ (alcohols,peroxides))} + (1 \times O-(C)(O)) + (1 \times O-(H)(O)) + (3 \times -CH_3 \text{ corr (quaternary))}$	<i>n</i> -Hexyl-3-hydroperoxide $C_6H_{14}O_2$ (2×C-(H) ₃ (C)) + (3×C-(H) ₂ (C) ₂) + (1×C-(H)(O)(C) ₂ (alcohols,peroxides)) + (1×O-(C)(O)) + (1×O-(H)(O))
Literature – Calculated = Residual Reference	Literature - Calculated = Residual Reference
Gas phase $\Delta_t H^\circ = -245.90 - 246.97$ 1.07 64KOZ/RAB	Gas phase $\Delta_t H^\circ = -265.52$
Liquid phase $\Delta_t H^\circ = -293.60 -292.38 -1.22 64KOZ/RAB$	Liquid phase $\Delta_t H^\circ = -305.10 -325.26$ 20.16 56PRI/MUL
Solid phase $\Delta_t H^\circ = -301.02$	Solid phase $\Delta_t H^\circ = -346.29$
n-Hexyl-1-hydroperoxide $C_6H_{14}O_2$ $(1 \times O-(H)(O)) + (1 \times O-(C)(O)) + (1 \times C-(H)_2(O)(C)) +$ $(4 \times C-(H)_2(C)_2) + (1 \times C-(H)_3(C))$ Literature – Calculated = Residual Reference	n -Heptyl-1-hydroperoxide $C_7H_{16}O_2$ $(1 \times C - (H)_3(C)) + (5 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(O)(C)) + (1 \times O - (C)(O)) + (1 \times O - (H)(O))$
	Literature - Calculated = Residual Reference
Gas phase $\Delta_t H^\circ = -250.69$	Gas phase $\Delta_t H^\circ = -271.32$
Liquid phase $\Delta_t H^\circ = -299.62 -311.58$ 11.96 56PRI/MUL	Liquid phase $\Delta_t H^\circ = -343.00 -337.31 -5.69$ 56PRI/MUL
Solid phase $\Delta_t H^\circ = -332.88$	Solid phase $\Delta_t H^\circ = -362.29$
$\begin{array}{c} \textit{n-Hexyl-2-hydroperoxide} & C_6H_{14}O_2\\ (2\times C-(H)_3(C))+(3\times C-(H)_2(C)_2)+\\ (1\times C-(H)(O)(C)_2 \text{ (alcohols,peroxides))}+(1\times O-(C)(O))+\\ (1\times O-(H)(O))+(1\times -CH_3 \text{ corr (tertiary))} \\ \\ \text{Literature}-\text{Calculated}=\text{Residual} \qquad \text{Reference} \end{array}$	n -Heptyl-2-hydroperoxide $C_7H_{16}O_2$ $(2 \times C - (H)_3(C)) + (4 \times C - (H)_2(C)_2) + (1 \times C - (H)(O)(C)_2 \text{ (alcohols, peroxides)}) + (1 \times O - (C)(O)) + (1 \times O - (H)(O)) + (1 \times -CH_3 \text{ corr (tertiary)})$
	Literature - Calculated = Residual Reference
Gas phase $\Delta_t H^{\circ} = -267.78$	Gas phase $\Delta_t H^\circ = -288.41$
Liquid phase $\Delta_{\rm f} H^{\circ} = -310.12 - 327.44$ 17.32 56PRI/MUL	Liquid phase $\Delta_t H^\circ = -346.20 -353.17$ 6.97 56PRI/MUL
Solid phase $\Delta_t H^{\circ} = -348.63$	Solid phase $\Delta_I H^{\circ} = -378.04$

TABLE 23. Hydroperoxides (9) - Continued

TABLE 24. Peroxyacids (8)

n-Heptyl-3-hydroperoxide $C_7H_{16}O_2$ $(2 \times C - (H)_3(C)) + (4 \times C - (H)_2(C)_2) +$ $(1 \times C - (H)(O)(C)_2 \text{ (alcohols, peroxides)}) + (1 \times O - (C)(O)) +$ $(1 \times O - (H)(O))$	$\begin{array}{c} \text{Perbenzoic acid} & C_7 H_6 O_3 \\ (1 \times C_B (CO)(C_B)_2) + (1 \times CO (O)(C_B)) + (1 \times O (CO)(O)) + \\ (1 \times O (H)(O)) + (5 \times C_B (H)(C_B)_2) \end{array}$
Literature - Calculated = Residual Reference	Literature – Calculated = Residual Reference
Gas phase $\Delta_t H^\circ = -286.15$	Gas phase $\Delta_t H^{\circ} = -200.71$
Liquid phase $\Delta_t H^{\circ} = -346.81 -350.99$ 4.18 56PRI/MUL	Liquid phase $\Delta_t H^{\circ} = -280.45$
Solid phase $\Delta_t H^\circ = -375.70$	Solid phase $\Delta_t H^\circ = -367.00 -290.00 -77.00$ 54BRI/DEC
n -Heptyl-4-hydroperoxide $C_7H_{16}O_2$ $(2 \times C - (H)_3(C)) + (4 \times C - (H)_2(C)_2) + (1 \times C - (H)(O)(C)_2 \text{ (alcohols, peroxides)}) + (1 \times O - (C)(O)) + (1 \times O - (H)(O))$	Perdodecanoic acid; Peroxylauric acid $C_{12}H_{24}O_3$ $(1\times C-(H)_3(C))+(9\times C-(H)_2(C)_2)+(1\times C-(H)_2(CO)(C))+$ $(1\times CO-(C)(O))+(1\times O-(CO)(O))+(1\times O-(H)(O))$ Literature – Calculated = Residual Reference
Literature - Calculated = Residual Reference	Gas phase $\Delta_t H^{\circ} = -547.27$
Gas phase $\Delta_t H^\circ = -286.15$	Liquid phase
Liquid phase $\Delta_1 H^{\circ} = -333.80 - 350.99$ 17.19 56PRI/MUL	$\Delta_t H^\circ = -644.44$ Solid phase
Solid phase $\Delta_t H^{\circ} = -375.70$	$\Delta_t H^\circ = -680.30 -678.73 -1.57$ 64SWA/SIL
1-Methyl-1-phenylethyl hydroperoxide; Cumyl hydroperoxide C ₂ H ₁₂ O ₂	Pertetradecanoic acid; Peroxymyristic acid $C_{14}H_{28}O_3$ $(1 \times C - (H)_3(C)) + (11 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) + (1 \times CO - (C)(O)) + (1 \times O - (CO)(O)) + (1 \times O - (H)(O))$
(5 × C _B -(H)(C _B) ₂) + (1 × C _B -(C)(C _B) ₂) + (1 × C-(C) ₂ (O)(C _B)) + (2 × C-(H) ₃ (C)) + (2 × -CH ₃ corr (quaternary)) + (1 × O-(C)(O)) + (1 × O-(H)(O))	Literature - Calculated = Residual Reference
Literature – Calculated = Residual Reference	Gas phase $\Delta_t H^\circ = -588.53$
Gas phase $\Delta_! H^{\circ} = -78.40 - 78.66$ 0.26 64KOZ/RAB	Liquid phase $\Delta_t H^\circ = -695.90$
Liquid phase $\Delta_t H^{\circ} = -143.49$	Solid phase $\Delta_t H^{\circ} = -749.90 -737.55 -12.35$ 64SWA/SIL
Solid phase $\Delta_t H^{\circ} = -161.80 - 161.83 0.03 64 \text{KOZ/RAB}$	

 $C_{16}H_{32}O_{3}$

C18H36O3

TABLE 24. Peroxyacids (8) - Continued

Gas phase $\Delta_t H^\circ =$

Liquid phase $\Delta_t H^\circ = -688.80$

-594.96

-670.73

-18.07

64SWA/SIL

TABLE 24. Peroxyacids (8) - Continued

Perhexadecanoic acid; Peroxypalmitic acid $(1 \times C - (H)_3(C)) + (13 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2) + (1$		(4×C-(I (1×O-(C)(O))+(1:	× C-(O)(C) ₃	(ethers,esters)) + (1 × CO-(0 ₁₂ (C) ₂) +	
Literature - Calculated = Residual	leference		3 corr (quat		2(-)2)	
Gas phase			Literatur	re – Calculateo	d = Residual	Reference
$\Delta_t H^\circ = -629.79$		Gas phase $\Delta_t H^\circ =$		- 626.72		
Liquid phase $\Delta_t H^\circ = -747.36$		Liquid pha	se			
Solid phase $\Delta_t H^\circ = -801.90 -796.37 -5.53 6$	4SWA/SIL	$\Delta_t H^\circ =$		-721.40	- 16.90	64SWA/SIL
Peroctadecanoic acid; Peroxystearic acid	C ₁₈ H ₃₆ O ₃	(4×C-(I		\times C-(O)(C) ₃	(ethers,esters)) + (1 × CO-(C	
$(1 \times C - (H)_3(C)) + (15 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)_2) + (1 \times C $)(C))+	(1×C-(H)+(11×C-(H ernary))	() ₂ (C) ₂)+	
$(1 \times CO - (C)(O)) + (1 \times O - (CO)(O)) + (1 \times O - (H)(O))$)(C))+	(1×C-(H	H) ₂ (CO)(C)) 3 corr (quat			Reference
$(1 \times CO - (C)(O)) + (1 \times O - (CO)(O)) + (1 \times O - (H)(O))$ $Literature - Calculated = Residual$)(C))+	(1×C-(H	H) ₂ (CO)(C)) 3 corr (quat	ernary))		Reference
$(1 \times \text{CO-(C)(O)}) + (1 \times \text{O-(CO)(O)}) + (1 \times \text{O-(H)(O)})$ $\text{Literature - Calculated = Residual}$ Gas phase $\Delta_{l}H^{\circ} = -671.05$)(C))+	(1×C-(I (3×-CH	H) ₂ (CO)(C)) 3 corr (quat Literatur	ernary)) e – Calculated		Reference 64SWA/SIL
$(1 \times \text{CO-(C)(O)}) + (1 \times \text{O-(CO)(O)}) + (1 \times \text{O-(H)(O)})$ $\text{Literature - Calculated = Residual} \qquad \text{R}$ Gas phase $\Delta_{\ell} H^{\circ} = \qquad -671.05$ Liquid phase $\Delta_{\ell} H^{\circ} = \qquad -798.82$ Solid phase)(C))+	$(1 \times C - (H + (1 \times C - (H + (1 \times C + (H + (1 \times C + (H + $	H) ₂ (CO)(C)) 3 corr (quat Literatur	e – Calculated – 667.98	i = Residual	
$(1 \times \text{CO-(C)(O)}) + (1 \times \text{O-(CO)(O)}) + (1 \times \text{O-(H)(O)})$ $\text{Literature - Calculated = Residual} \qquad \text{R}$ Gas phase $\Delta_{\ell} H^{\circ} = \qquad -671.05$ Liquid phase $\Delta_{\ell} H^{\circ} = \qquad -798.82$ Solid phase	eference	$(1 \times C - (H + (1 \times C - (H + (1 \times C + (H + (1 \times C + (H + $	H) ₂ (CO)(C)) 3 corr (quat Literatur	e – Calculated – 667.98	i = Residual	
$(1 \times \text{CO-(C)(O)}) + (1 \times \text{O-(CO)(O)}) + (1 \times \text{O-(H)(O)})$ $\text{Literature - Calculated = Residual} \qquad \text{R}$ Gas phase $\Delta_t H^\circ = \qquad -671.05$ Liquid phase $\Delta_t H^\circ = \qquad -798.82$ Solid phase $\Delta_t H^\circ = \qquad -857.30 \qquad -855.19 \qquad -2.11 \qquad 6$	4SWA/SIL	$(1 \times C - (H + (1 \times C - (H + (1 \times C + (H + (1 \times C + (H + $	H) ₂ (CO)(C)) 3 corr (quat Literatur	e – Calculated – 667.98	i = Residual	

TABLE	25.	Carbonates	(3)
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TABLE 26. Amines (50)

Diethyl carbonate $(2 \times C - (H)_3(C))$ $(1 \times CO - (O)_2)$	+(2×0	C-(H) ₂ (O)(C	C))+(2×O-(C	C ₅ H ₁₀ O ₃ C)(CO))+	Aminometh (1×C-(F		l amine ×N-(H) ₂ (C)),	$\sigma = 3$	CH ₅
()-/	rature -	- Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = -637.$	90	639.94	2.04	72MAN	Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$	-23.01 50.08 242.59	-23.01 50.08 242.59	0.00 0.00 0.00	37AST/SIL 69STU/WES 69STU/WES
Liquid phase $\Delta_t H^\circ = -681$ $C_p^\circ = 210$	-	-680.86 210.86	- 0.64 0.04	72MAN2 34KOL/UDO	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-185.33 32.25 -13.01		
					Liquid phas	se			
Solid phase					$\Delta_l H^\circ =$	-47.27	- 47.28	0.01	90CHA/GAD
$\Delta_t H^\circ =$		-703.68			$C_p^{\circ} =$	102.09	99.07	3.02	90CHA/GAD
$C_p^{\circ} =$		170.99			S° =	150.43	155.01	-4.58	90CHA/GAD
$S^{\circ} = \Delta_{f}S^{\circ} =$		144.10 -845.02			$\Delta_f S^\circ = \Delta_f G^\circ =$		- 272.91 34.09		
$\Delta_{f}G^{\circ} =$		- 451.74			$lnK_{f} =$		13.75		
$\ln K_{\rm f} =$		182.23							
Diphenyl carbons	ite			C ₁₃ H ₁₀ O ₃	Aminoethai (1×C-(F		nine × N-(H)2(C)) -	+ (1 × C−(H)₂(C_2H_7 $C)(N)), \sigma = 3$
$(10 \times C_{B}-(H))(0)$ $(1 \times CO-(O)_{2})$	$(C_B)_2$ + ($2 \times C_B - (O)(C$	$(C_B)_2$) + (2 × O-	$+(C_B)(CO))+$		**	re – Calculated		Reference

(200	(-)2)				
	Literature - Calculated = Residual				
Gas phase Δ _t H° =	-311.30	-317.28	5.98	71CAR/FIN	
Liquid pha	ase -377.70	-382.62	4.92	71CAR/FIN	
Solid phas	se	<u>.</u>			
-	-401.20	- 395.70	-5.50	58SIN/HIL	
$C_p^{\circ} =$	263.13	263.13	0.00	58SIN/HIL	
S° =	278.40	278.40	0.00	58SIN/HIL	
$\Delta_6 S^\circ =$		<i>−756.64</i>			
$\Delta_{r}G^{\circ} =$		-170.11			
$lnK_f =$		68.62			

1,3-Dioxolan-2-one; Ethylene carbonate	C ₃ H ₄ O ₃
$(2 \times C - (H)_2(O)(C)) + (2 \times O - (C)(CO)) + (1 \times CO - (O)_2) +$	
(1 × Ethyl carbonate rsc)	

	Litera	ture-Calculated	Reference		
Solid phas $\Delta_t H^\circ =$		- 586.30	0.00	83CAL	

	Literatu	Reference		
Gas phase $\Delta_t H^\circ =$	- - 47.47	51.31	3.84	90CHA/GAD
$C_n^{\circ} =$	72.63	72.76	-0.13	69STU/WES
S° –	284.85	284.85	0.00	69STU/WES
Δ ₆ S° =	20	- 279.38	0.00	0,010,1120
$\Delta_i G^\circ =$		31.99		
$lnK_f =$		- 12.90		
Liquid pha	ase			
	-74.13	-78.08	3.95	90CHA/GAD
C _p -		129.49		
S° =		187.39		
$\Delta_f S^\circ =$		-376.84		
$\Delta_{\rm f}G^{\circ} =$		34.27		
lnK_t -		-13.83		

1-Aminopropane; n -Propyl amine C_3H_9N $(1 \times C(H)_3(C)) + (1 \times C(H)_2(C)_2) + (1 \times C(H)_2(C)(N)) + (1 \times N(H)_2(C)), \sigma = 3$										
	Literatur	e – Calculated =	Reference							
Gas phase										
$\Delta_f H^* =$	- 70.10	-71.94	1.84	90CHA/GAD						
$C_p^{\circ} =$	95.77	95.65	0.12	69STU/WES						
S° =	324.18	324.01	0.17	69STU/WES						
$\Delta_f S^\circ =$		-376.53								
$\Delta_f G^\circ =$		40.32								
$lnK_f =$		-16.27								

	Literature	e – Calculated =	= Residual	Reference		Literature - Calculated = Residual		Reference	
Liquid phas	e				Gas phase				
	- 101.47	- 103.81	2.34	90CHA/GAD	$\Delta_i H^{\circ} =$		- 133.83		
$C_p^{\circ} =$	162.54	159.91	2.63	90CHA/GAD	$C_p^{\circ} =$		164.32		
S° =	227.44	219.77	7.67	90CHA/GAD	S° =		441.49		
$\Delta_f S^\circ =$		- 480.77			$\Delta_f S^\circ =$		-667.99		
$\ln G^{\circ} = \ln K_{c} =$		39.53 - 15.95			$\Delta_f G^\circ = \ln K_f =$		65.33 - 26.35		
niwt –									
					Liquid pha	se			
	ane; n -Buty			C ₄ H ₁₁ N	$\Delta_t H^\circ =$	050.00	-181.00	0.00	
		× C-(H)2(C)2) +	F(I×C-(H) ₂ ((C)(N))+	$C_p^{\circ} = S^{\circ} =$	252.00	251.17	0.83	71KON/WAD
(1 × N-();	$H_{2}(C)$, $\sigma =$	٠ ٥			$\Delta_{f}S^{\circ} =$		316.91 - 792.56		
	T itaratus	e – Calculated =	= Residual	Reference	$\Delta_{\mathbf{f}} S^{\circ} = \Delta_{\mathbf{f}} G^{\circ} =$		- 792.36 55.30		
	Piteratul	- Calculated =	- Mojuudi	Kelefelle	$\ln K_{\rm f} =$		- 22.31		
Sas phase	- 92.00	- 92.57	0.57	69WAD					
$C_p^{\circ} =$	118.53	118.54	-0.01	69STU/WES					
S° =	363.00	363.17	-0.17	69STU/WES	2-Methylpr	opyl amine:	Isobutyl amino	2	C4H11
$\Delta_i S^o =$	202.00	-473.68					\times C-(H)(C) ₃)+		
$\Delta_i G^{\circ} =$		48.66					$+(1\times N-(H)_2(C))$		(,))
$lnK_i =$		- 19.63			` `	/=(/(//	()2(-	,,	
						Literatu	re – Calculated :	= Residual	Reference
iquid phas Δ _τ Η° =	se 127.70	- 129.54	1.84	59EVA/FAI	Gas phase				
$C_p^{\circ} =$	188.00	190.33	-2.33	71KON/WAD	$\Delta_t H^\circ =$	-98.80	- 99.26	0.46	69WAD
S° =	100.00	252.15		, , , , , , , , , , , , , , , , , , , ,	$C_p^{\circ} =$	70.00	118.57	00	07111111
$\Delta_f S^\circ =$		- 584.70			- p				
Δ ₁ G° =		44.79							
$lnK_f =$		-18.07			Liquid pha	se			
	······································				$\Delta_{f}H^{\circ} =$	- 132.60	- 134.82	2.22	70GOO/MOO
					$C_{\rho}^{\circ} =$	194.00	187.35	6.65	71KON/WAD
				~	S° =		246.80		
-	itane; n-Pei	•		C ₅ H ₁₃ N	$\Delta_f S^\circ =$		- 590.05		
		\times C-(H) ₂ (C) ₂) +	F(1×C-(H) ₂ (C)(N))+	$\Delta_{\rm f}G^{\circ} =$		41.10		
(1×N-(F	·I) ₂ (C)), σ =	= 3			$lnK_f =$		- 16.58		
	Literatur	e – Calculated =	= Residual	Reference					
Gas phase					1,2-Ethanediamine; Ethylenediamine $(2 \times C - (H)_2(C)(N)) + (2 \times N - (H)_2(C)), \sigma = 18$				C ₂ H ₈ N
$\Delta_f H^\circ =$		113.20			, - (-				
00		141.43				Literatur	e – Calculated =	= Residual	Reference
$C_p^{\circ} =$		402.33							
S° =		- 570.84							
S° = Δ _t S° =		56.99			Gas phase				
$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = 0$		22.99			$\Delta_t H^\circ =$	-17.60	-18.10	0.50	69WAD
S° =					$C_p^{\circ} =$		94.06		
$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = 0$					s° =	321.80	309.29	12.51	75MES/FIN
$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = -\infty$									
$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = 1$ $\Delta_{t}G^{\circ} = 1$:e	155.05			$\Delta_{\rm f}S^{\circ} =$		-415.98		
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1}{2}$ iquid phas		-155.27 220.75	0.75	71VONAVA P	$\Delta_{f}G^{\circ} =$		105.92		
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = $ iquid phas $\Delta_t H^{\circ} = C_p^{\circ} = $	se 218.00	220.75	-2.75	71KON/WAD					
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \ln K_t = \frac{\Delta_t H^{\circ}}{\Delta_t H^{\circ}} = \frac{C_p^{\circ}}{S^{\circ}} = \frac{S^{\circ}}{\Delta_t H^{\circ}} = \frac{C_p^{\circ}}{\Delta_t H^{\circ}} = \frac{C_p^{\circ}}{S^{\circ}} = \frac{C_p^{\circ}}{\Delta_t H^{\circ}} = \frac{C_p^{\circ}}{\Delta$		220.75 284.53	- 2.75	71KON/WAD	$\Delta_{f}G^{\circ} =$		105.92		
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = -\frac{1}{2}$ iquid phas $\Delta_t H^{\circ} = C_p^{\circ} = -\frac{1}{2}$		220.75	-2.75	71KON/WAD	$\Delta_{f}G^{\circ} =$	·····	105.92		

TABLE 26.	Amines	(50) -	Continued
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TABLE 26. Amines (50) - Continued			TABLE	26. Amines (5	0) – Contin	ued
1,2-Ethanediamine; Ethylenediamine (Continued) $(2 \times C - (H)_2(C)(N)) + (2 \times N - (H)_2(C)), \sigma = 18$	C ₂ H ₈ N ₂	2-Aminopro (1×N-(F (2×-CH)		× C-(H) ₃ (C))	+ (1 × C-(H)(0	C ₃ H ₉ N C) ₂ (N)) +
Literature - Calculated = Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Liquid phase						
$\Delta_{t}H^{\circ} = -63.00 -60.94 -2.06$ $C_{p}^{\circ} = 172.59 186.02 -13.43$ $S^{\circ} = 202.42 208.18 -5.76$ $\Delta_{t}S^{\circ} = -517.08$ $\Delta_{t}G^{\circ} = 93.23$	70GOO/MOO 75MES/FIN 75MES/FIN	Gas phase $\Delta_t H^\circ = C_p^\circ =$	-83.70	- 86.49 94.43	2.79	90CHA/GAD
$\ln K_{\rm f} = -37.61$		Liquid phas	se			
1,2-Propanediamine $(1 \times C - (H)_2(C)(N)) + (2 \times N - (H)_2(C)) + (1 \times C - (H)_3(C) + (1 \times C - (H)_2(C)) + (1 \times C - (H)_3(C) + (1 \times C - (H)_3(C)) + (1 \times C $	C ₃ H ₁₀ N ₂ (C))+	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{f} = 0$	-112.30 163.85 218.32	-113.90 163.83 218.31 -482.23 29.88 -12.05	1.60 0.02 0.01	90CHA/GAD 72FIN/MES 72FIN/MES
Literature – Calculated = Residual	Reference					
Gas phase $\Delta_t H^\circ = -53.60 -51.02 -2.58$	69WAD	2-Aminobut (2×C-(H (1×-CH ₃	$I)_3(C)) + (1$	tyl amine × C-(H) ₂ (C) ₂) ary)) + (1 × N-	+ (1 × C-(H)((H) ₂ (C)), σ =	C ₄ H ₁₁ N C) ₂ (N)) + 9
$C_p^{\circ} = 115.73$			Literatur	e – Calculated	= Residual	Reference
Liquid phase $\Delta_t H^\circ = -97.80 -94.58 -3.22$ $C_\rho^\circ = 220.36$ $S^\circ = 239.10$ $\Delta_t S^\circ = -622.47$ $\Delta_t G^\circ = 91.01$ $\ln K_t = -36.71$	70GOO/MOO	Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 104.90 117.11 351.04	- 104.86 117.32 342.14 - 494.71 42.64 - 17.20	- 0.04 - 0.21 8.90	69WAD 69STU/WES 69STU/WES
1,2-Butanediamine $(2 \times N - (H)_2(C)) + (1 \times C - (H)_2(C)(N)) + (1 \times C - (H)_2(C)(N)) + (1 \times C - (H)_3(C)) + (1 \times C - (H)(C)_2(N))$ Literature — Calculated = Residual	$C_4H_{12}N_2$ $(C)_2) +$ Reference	Liquid phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ =$	e 137.49	-137.45 194.25 250.69 -586.16	-0.04	59EVA/FAI
		$\Delta_f G^\circ = In K_f =$		37.31 -15.05		
Gas phase $\Delta_t H^\circ = -74.00 - 69.39 - 4.61$ $C_c^\circ = 138.62$	70GOO/MOO					٠
Liquid phase $\Delta_t H^o = -120.20 -118.13 -2.07$	70GOO/MOO	(3×C-(H	() ₃ (C)) + (1) corr (quat	nne; tert-Butyl × N-(H) ₂ (C)) + ernary)), $\sigma =$	+ (1 × C−(C)₃(1 81	
$C_p^{\circ} = 250.78$ $S^{\circ} = 271.48$ $\Delta_p S^{\circ} = -726.41$			Literatur	e – Calculated	= Residual	Reference
$ \begin{array}{rcl} \Lambda_t G^{\circ} &=& 98.45 \\ \ln K_t &=& -39.71 \end{array} $		Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_t =$	- 121.00 119.96 337.10	- 120.92 119.95 317.23 - 519.62 34.00 - 13.72	-0.08 0.01 19.87	69WAD 69STU/WES 69STU/WES

(3×C-(H	$(1)_3(C) + (1)_3(C)$	ne; tert-Butyl $< N-(H)_2(C)$) + ernary)), $\sigma =$	- (1 × C-(C) ₃ (1	nued) $C_4H_{11}N$ N))+	Diethylami (2×C-(F	H) ₃ (C)) + (2	2×C-(H) ₂ (C)(1		$C_4H_{11}N$ $H)(C)_2), \sigma = 9$
		e – Calculated	-	Reference	· · · · · · · · · · · · · · · · · · ·	Literatu	re – Calculated	= Residual	Reference
Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	e -150.60 191.71 233.63	-150.57 191.69 233.62 -603.23 29.28 -11.81	-0.03 0.02 0.01	67SMI/GOO 72FIN/MES 72FIN/MES	Gas phase $\Delta_{\ell}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \ln K_{\ell} = \ln K_{\ell} = 0$	-72.50 103.81 352.21	-73.57 109.10 354.85 -482.00 70.14 -28.29	1.07 - 5.29 - 2.64	69WAD 69STU/WES 69STU/WES
	I) ₂ (C))+(1 corr (quat	iamine × C-(H) ₂ (C)(N ernary)) + (1 × e – Calculated	C-(C)3(N))	$C_4H_{12}N_2$ $H)_3(C)) +$ Reference	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = 0$	se 103.70	- 105.32 193.17 263.45 - 573.40 65.64 - 26.48	1.62	58JAF
Gas phase $\Delta_t H^\circ = C_p^\circ =$	-90.20	-83.15 141.25	-7.05	70GOO/MOO			$2 \times C - (H)_2(C)_2$ = 9	+ (2 × C-(H) ₂ (C ₆ H ₁₅ N (C)(N)) +
Liquid phas $\Delta_t H^\circ =$	se 133.90	- 129.04	-4.86	70GOO/MOO		Literatu	re – Calculated –––––	= Residual 	Reference
$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f = -$		248.22 254.41 -743.48 92.63 -37.37		CHN	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-116.10	- 114.83 154.88 433.17 - 676.30 86.81 - 35.02	-1.27	69WAD
Dimethylan (2×C-(I		\times N-(H)(C) ₂),	$\sigma = 9$	C ₂ H ₇ N	· · · · · · · · · · · · · · · · · · ·				
Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ =$		- 16.97 63.74 270.33		Reference 39AST/EID 69STU/WES 69STU/WES	Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	se 156.11	156.78 254.01 328.21 781.26 76.15 30.72	0.67	71LEB/KAT
$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$		- 293.90 70.66 - 28.50				$-1)_3(C))+(2$	×C-(H)(C) ₂ (N		C ₆ H ₁₅ N
Liquid pha $\Delta_t H^\circ = C_p^\circ =$	se -43.90	-43.72 132.33	-0.18	58JAF	(4×-CH		iary)) + (1 × N- re – Calculated		Reference
$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$		198.69 - 365.54 65.27 - 26.33			Gas phase $\Delta_f II^\circ = C_p^\circ =$	144.00	143.93 152.44	-0.07	69WAD

TABLE 26. Amines (50) - Continued

Diisopropylamine C_6H_{12} $(4 \times C-(H)_3(C)) + (2 \times C-(H)(C)_2(N)) + (4 \times -CH_3 \text{ corr (tertiary)}) + (1 \times N-(H)(C)_2)$	N n-Butylisobutylamine $(3 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)_3)$ $(2 \times -CH_3 \text{ corr (tertiary)}) + (2 \times C - (H)_2(C)(N)) +$ $(1 \times N - (H)(C)_2)$	C ₈ H ₁₉ N +
Literature - Calculated = Residual Reference	_ Literature - Calculated = Residual	Reference
Liquid phase $\Delta_t H^\circ = -178.50 -176.96 -1.54$ 71LEB/KAT $C_p^\circ = 261.85$ $S^\circ = 325.29$ $\Delta_t S^\circ = -784.18$ $\Delta_t G^\circ = 56.84$	Gas phase $\Delta_t H^\circ = -171.00 - 162.78 - 8.22$ $C_p^\circ = 200.69$	62BED/EDM
$\begin{aligned} &\ln K_{\rm f} = & -22.93 \\ &\text{Di-n-butylamine} & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & $	$C_{p}^{\circ} = 311.87$ $S^{\circ} = 387.62$	52BED/EDM
Literature - Calculated = Residual Reference	_	
Gas phase $\Delta_t H^{\circ} = -156.61 - 156.09 -0.52$ 69WAD $C_p^{\circ} = 200.66$	Trimethylamine $(3 \times C-(H)_3(C)) + (1 \times N-(C)_3) + (3 \times -CH_3 \text{ corr (quaternary))}, \sigma = 81$	C ₃ H ₉ N
$S^{\circ} = 511.49$ $\Delta_t S^{\circ} = -870.60$ $\Delta_t G^{\circ} = 103.48$ $\ln K_t = -41.74$	Literature – Calculated = Residual Gas phase	Reference
Liquid phase $ \Delta_t H^{\circ} = -206.00 -208.24 2.24 71LEB/KAT $ $ C_p^{\circ} = 314.85 $ $ S^{\circ} = 392.97 $ $ \Delta_t S^{\circ} = -989.12 $	$C_p^{\circ} = 91.76 92.29 -0.53 4$	I4AST/SAG I4AST/SAG I4AST/SAG
$\Delta_{\rm f}G^{\circ} = 86.67$ $\ln K_{\rm f} = -34.96$ Diisobutylamine $C_{\rm g}H_{\rm f}$	$C_p^{\circ} = 135.55$ $S^{\circ} = 211.28$	8JAF
$(4 \times C - (H)_3(C)) + (2 \times C - (H)(C)_3) + (4 \times -CH_3 \text{ corr (tertiary)}) + (2 \times C - (H)_2(C)(N)) + (1 \times N - (H)(C)_2)$	$\Delta_1 G^\circ = 101.87$ $\ln K_1 = -41.09$	
Literature – Calculated = Residual Reference	_	
Gas phase $\Delta_l H^{\circ} = -179.20 - 169.47 - 9.73$ 71LEB/KAT $C_p^{\circ} = 200.72$	Triethylamine $(3 \times C - (H)_3(C)) + (3 \times C - (H)_2(C)(N)) + (1 \times N - (C)_3),$ Literature – Calculated = Residual	$C_6H_{15}N$ $\sigma = 81$ Reference
Liquid phase $ \Delta_{l}H^{\circ} = -218.50 \qquad -218.80 \qquad 0.30 \qquad 71 LEB/KAT $ $ C^{\circ}_{l} = \qquad 308.89 \qquad 0.30 \qquad 71 LEB/KAT $ $ S^{\circ} = \qquad 382.27 \qquad 0.30 \qquad $	$C_p^{\circ} = 160.92 160.33 0.59 6$	99WAD 9STU/WES 9STU/WES

Triethylamine (Continued) $(3 \times C - (H)_3(C)) + (3 \times C - (H)_2(C)(N)) + (1 \times N - (C)$	$C_6H_{15}N$ $\sigma = 81$	Tri-n-hexylamine $(3 \times C - (H)_3(C)) + (1 \times N - (C)_3), \sigma =$	$(12 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2)$	$C_{18}H_{39}N_{2}(C)(N)) +$
Literature – Calculated = Residual	Reference	, , , , , ,	ure – Calculated = Residual	Reference
Liquid phase				
Liquid phase $\Delta_t H^\circ = -127.70 -123.23 -4.47$ $C_p^\circ = 226.81$ $S^\circ = 308.42$	66LEB	Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 342.74 435.01	
$\Delta_{t}S^{\circ} = -801.05$		S° =	880.41	
$\Delta_t G^{\circ} = 115.60$		$\Delta_{\rm f}S^{\circ} =$	– 1864.79	
$\ln K_{\rm f} = -46.63$		$\Delta_t G^{\circ} =$	213.25	
		$lnK_f =$	-86.02	
Tri a manulamina	C ₉ H ₂₁ N	Liquid phase		
Tri-n-propylamine $(3 \times C - (H)_3(C)) + (3 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2)$		$\Delta_t H^\circ = -433.00$	-431.99 -1.01	66LEB
$(1 \times N - (C)_3), \sigma = 81$	-)(- ·)) ·	$C_p^{\circ} =$	591.85	
(2000) (2)3), 2		S° =	696.98	
Literature - Calculated = Residual	Reference	$\Delta_{f}S^{\circ} =$	- 2048.22	
		$\Delta_f G^{\circ} =$	178.69	
Gas phase		$lnK_f =$	−72.08	
Gas phase $\Delta_t H^{\circ} = -161.00 - 157.07 - 3.93$	69WAD			
$C_p^{\circ} = 229.00$		material and a		a
S° = 527.97		Tri-n -octylamine	(19.40 (II) (O)) ((0.40 (II)	C24H51N
$\Delta_{\rm f} S^{\circ} = -990.43$			$(18 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2)$	₂ (C)(N))+
$\Delta_t G^{\circ} = 138.23$ $\ln K_t = -55.76$		$(1 \times N - (C)_3), \sigma =$	01	
$\ln K_{\rm f} = -55.76$		Literat	ure - Calculated = Residual	Reference
Liquid phase				
$\Delta_t H^\circ = -207.11 -200.42 -6.69$	66LEB	Gas phase		
$C_p^{\circ} = 318.07$		$\Delta_{\rm f}H^{\circ} =$	- 466.52	
$S^{\circ} = 405.56$		$C_{\rho}^{\circ} =$	572.35	
$\Delta_t S^\circ = -1112.85$		S° =	1115.37	
$\Delta_{\rm f}G^{\circ} = 131.37$		$\Delta_{\mathbf{r}} S^{\circ} =$	-2447.70	
$\ln K_{\rm f} = -53.00$		$\Delta_f G^{\circ} = \ln K_f =$	263.26 106.20	
		musi —		
			100.20	
Tri-n-butylamine	C ₁₂ H ₂₇ N	Liquid phase		
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2)$		Liquid phase $\Delta_t H^\circ = -585.01$	- 586.37 1 .3 6	66LEB
•		Liquid phase $\Delta_t H^{\circ} = -585.01$ $C_p^{\circ} =$	- 586.37 1.36 774.37	66LEB
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_3)$	C)(N))+	Liquid phase $\Delta_t H^o = -585.01$ $C_p^o = S^o =$	- 586.37 1.36 774.37 891.26	66LEB
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2)$		Liquid phase $\Delta_t H^\circ = -585.01$ $C_p^\circ = S^\circ = \Delta_t S^\circ =$	- 586.37 1.36 774.37 891.26 - 2671.81	66LEB
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_3)$	C)(N))+	Liquid phase $ \Delta_t H^\circ = -585.01 $ $ C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = 0 $	- 586.37 1.36 774.37 891.26 - 2671.81 210.23	66LEB
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) +$	C)(N))+	Liquid phase $\Delta_t H^\circ = -585.01$ $C_p^\circ = S^\circ = \Delta_t S^\circ =$	- 586.37 1.36 774.37 891.26 - 2671.81	66LEB
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_3)$	C)(N))+	Liquid phase $ \Delta_t H^\circ = -585.01 $ $ C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = 0 $	- 586.37 1.36 774.37 891.26 - 2671.81 210.23	66LEB
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2)$ $(1 \times N - (C)_3)$ Literature – Calculated = Residual Gas phase	C)(N))+	Liquid phase $ \Delta_t H^\circ = -585.01 $ $ C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = 0 $	- 586.37 1.36 774.37 891.26 - 2671.81 210.23	66LEB
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2)$ $(1 \times N - (C)_3)$ Literature – Calculated = Residual Gas phase $\Delta_t H^\circ = -218.96$	C)(N))+	Liquid phase $\Delta_t H^\circ = -585.01$ $C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = -585.01$ Tri-n-nonylamine	-586.37 1.36 774.37 891.26 -2671.81 210.23 -84.81	C ₂₇ H ₅₇ N
$(3 \times C^{-}(H)_{3}(C)) + (6 \times C^{-}(H)_{2}(C)_{2}) + (3 \times C^{-}(H)_{2}(C)_{2})$ $(1 \times N^{-}(C)_{3})$ Literature – Calculated = Residual Gas phase $\Delta_{t}H^{\circ} = -218.96$ $C_{n}^{\circ} = 297.67$	C)(N))+	Liquid phase $\Delta_t H^\circ = -585.01$ $C_\rho^\circ = S^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = InK_f = $ Tri- <i>n</i> -nonylamine $(3 \times C - (H)_3(C)) + 6$	-586.37 1.36 774.37 891.26 -2671.81 210.23 -84.81	C ₂₇ H ₅₇ N
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) +$	Reference	Liquid phase $\Delta_t H^\circ = -585.01$ $C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = -585.01$ Tri-n-nonylamine	-586.37 1.36 774.37 891.26 -2671.81 210.23 -84.81	C ₂₇ H ₅₇ N
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) +$	C)(N))+	Liquid phase $\Delta_{t}H^{\circ} = -585.01$ $C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Tri- <i>n</i> -nonylamine $(3 \times C - (H)_{3}(C)) + (1 \times N - (C)_{3}), \sigma = 0$	$ \begin{array}{rcl} -586.37 & 1.36 \\ 774.37 & 891.26 \\ -2671.81 & 210.23 \\ -84.81 \end{array} $ $ \begin{array}{rcl} (21 \times C - (H)_2(C)_2) + (3 \times C - (H)_{81}) \end{array} $	C27H57N 2(C)(N)) +
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) +$	Reference	Liquid phase $\Delta_{t}H^{\circ} = -585.01$ $C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Tri- <i>n</i> -nonylamine $(3 \times C - (H)_{3}(C)) + (1 \times N - (C)_{3}), \sigma = 0$	-586.37 1.36 774.37 891.26 -2671.81 210.23 -84.81	C ₂₇ H ₅₇ N
$(3 \times C - (H)_{3}(C)) + (6 \times C - (H)_{2}(C)_{2}) + (3 \times C - (H)_{2}(C)_{2}) + (3 \times C - (H)_{2}(C)_{2}) + (3 \times C - (H)_{2}(C)_{2$	Reference	Liquid phase $\Delta_{t}H^{\circ} = -585.01$ $C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Tri- <i>n</i> -nonylamine $(3 \times C - (H)_{3}(C)) + (1 \times N - (C)_{3}), \sigma = 0$	$ \begin{array}{rcl} -586.37 & 1.36 \\ 774.37 & 891.26 \\ -2671.81 & 210.23 \\ -84.81 \end{array} $ $ \begin{array}{rcl} (21 \times C - (H)_2(C)_2) + (3 \times C - (H)_{81}) \end{array} $	C27H57N 2(C)(N)) +
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) +$	Reference	Liquid phase $\Delta_{f}H^{\circ} = -585.01$ $C_{\rho}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{f}G^{\circ} = InK_{f} = S^{\circ} = InK_{f} = InK$	$ \begin{array}{rcl} -586.37 & 1.36 \\ 774.37 & 891.26 \\ -2671.81 & 210.23 \\ -84.81 \end{array} $ $ \begin{array}{rcl} (21 \times C - (H)_2(C)_2) + (3 \times C - (H)_{81}) \end{array} $	C27H57N 2(C)(N)) +
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) +$	Reference	Liquid phase $\Delta_{t}H^{\circ} = -585.01$ $C^{\circ}_{\rho} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = $ $Tri-n-nonylamine$ $(3 \times C-(H)_{3}(C)) + (1 \times N-(C)_{3}), \sigma = $ Literat Gas phase	$-586.37 1.36$ 774.37 891.26 -2671.81 210.23 -84.81 $(21 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2)$ 81 $ure - Calculated = Residual$	C27H57N 2(C)(N)) +
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) +$	Reference	Liquid phase $\Delta_{t}H^{\circ} = -585.01$ $C^{\circ}_{\rho} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = $ $Tri-n-nonylamine$ $(3 \times C-(H)_{3}(C)) + (1 \times N-(C)_{3}), \sigma = $ $Literat$ $Gas phase$ $\Delta_{t}H^{\circ} = $	$-586.37 1.36$ 774.37 891.26 -2671.81 210.23 -84.81 $(21 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2)$ $ure - Calculated = Residual$ -528.41	C27H57N 2(C)(N)) +
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) +$	Reference	Liquid phase $\Delta_{t}H^{\circ} = -585.01$ $C^{\circ}_{\rho} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{3 \times C - (H)_{3}(C) + (1 \times N - (C)_{3}), \sigma = \frac{Literat}{Gas phase}$ $\Delta_{t}H^{\circ} = C^{\circ}_{\rho} = \frac{C}{\sigma}$	$-586.37 1.36$ 774.37 891.26 -2671.81 210.23 -84.81 $(21 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2)$ $ure - Calculated = Residual$ -528.41 641.02	C27H57N 2(C)(N)) +
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) +$	Reference	Liquid phase $\Delta_{t}H^{\circ} = -585.01$ $C^{\circ}_{\rho} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = 1nK_{f} = 1nK_{f}$	$-586.37 1.36$ 774.37 891.26 -2671.81 210.23 -84.81 $(21 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2)$ $ure - Calculated = Residual$ -528.41 641.02 1232.85	C27H57N 2(C)(N)) +
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) +$	Reference	Liquid phase $\Delta_{t}H^{\circ} = -585.01$ $C^{\circ}_{\rho} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \frac{1}{N}$ Tri-n-nonylamine $(3 \times C - (H)_{3}(C)) + (1 \times N - (C)_{3}), \sigma = \frac{1}{N}$ Literat Gas phase $\Delta_{t}H^{\circ} = C^{\circ}_{\rho} = S^{\circ} = \Delta_{t}S^{\circ} = \frac{1}{N}$	$-586.37 1.36$ 774.37 891.26 -2671.81 210.23 -84.81 $(21 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2)$ $ure - Calculated = Residual$ -528.41 641.02 1232.85 -2739.15	C27H57N 2(C)(N)) +
$(3 \times C - (H)_3(C)) + (6 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) +$	Reference	Liquid phase $\Delta_{t}H^{\circ} = -585.01$ $C^{\circ}_{\rho} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = 1nK_{f} = 1nK_{f}$	$-586.37 1.36$ 774.37 891.26 -2671.81 210.23 -84.81 $(21 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2) + (3 \times C - (H)_2(C)_2)$ $ure - Calculated = Residual$ -528.41 641.02 1232.85	C27H57N 2(C)(N)) +

TABLE 26. Amines (50) - Continued

Tri- <i>n</i> -nonylar (3 × C-(H); (1 × N-(C);	3(C))+(21	\times C-(H) ₂ (C) ₂)	+ (3×C-(H) ₂ ($C_{27}H_{57}N$ (C)(N)) +	Tribenzylamia (15 × C _B -(I (1 × N-(C)	$H)(C_B)_2) +$	$(3 \times C_B - (C))(C)$	$(C_B)_2$) + (3 × C-	$C_{21}H_{21}N$ $(H)_2(C_B)(N)) +$
	Literature	e – Calculated =	Residual	Reference		Literatur	e – Calculated	= Residual	Reference
$C_p^{\circ} =$: - 661.62	-663.56 865.63	1.94	66LEB	Gas phase $\Delta_t H^\circ =$		322.15		
$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f =$		988.40 2983.60 226.00 91.17			Liquid phase $\Delta_t H^\circ = C_p^\circ =$		213.61 455.98		
		4×C−(H)2(C)2)	+ (3×C-(H) ₂	C ₃₀ H ₆₃ N (C)(N)) +	Solid phase $\Delta_t H^\circ =$	140.70	140.72	-0.02	56TAV/LAM
(1001)	, . , .	e – Calculated =	= Residual	Reference	Cyclopropylar (2×C-(H); (1×Cyclop	$_{2}(C)_{2})+(1$	×C-(H)(C)₂(I	N))+(1×N-(C₃H ₇ N H)₂(C))+
Gas phase $\Delta_f H^\circ = C_p^\circ =$		-590.30 709.69				Literature	e – Calculated	= Residual	Reference
$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f =$		1350.33 -3030.60 313.27 -126.37			Gas phase $\Delta_t H^\circ = C_\rho^\circ =$	77.00	76.44 76.02	0.56	71GOO/MOO
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	e 738.02	-740.75 956.89 1085.54 -3295.40	2.73	66LEB	Liquid phase $\Delta_t H^\circ = C_p^\circ =$	45.80	45.80 123.18	0.00	71GOO/MOO
$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = $		241.77 - 97.53			Cyclobutylam (3×C-(H); (1×Cyclob	$_{2}(C)_{2})+(1$	×C-(H)(C)₂(l	N))+(1×N-(C₄H₃N H)₂(C))+
Triphenylam (15×C _B -(- (3 × C _B (N)) +	· (1 × N-(C _B) ₃)	C ₁₈ H ₁₅ N	· ·	Literature	e – Calculated	= Residual	Reference
	Literatui	re – Calculated :	= Residual	Reference	Gas phase $\Delta_t H^\circ =$	41.20	51.55	- 10.35	75GOO/MES
Gas phase $\Delta_t H^\circ =$	326.77	326.40	0.37	78STE	$C_p^{\circ} =$ Liquid phase		92.30		
Liquid phase $\Delta_t H^\circ =$	e 247.72	248.70	-0.98	78STE	$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	5.60	15.13 171.45 200.33 - 505.95	-9.53	75GOO/MES
Solid phase $\Delta_t H^\circ = C_p^\circ =$	234.72 301.70	234.70 301.95	0.02 - 0.25	78STE 78STE	$\Delta_f G^\circ = \\ \ln K_f = $		165.98 - 66.95		

		×C-(H)(C) ₂ (1 ub) rsc)	N))+(1×N-($C_5H_{11}N$ $H)_2(C)) +$		H)(C_B) ₂) +	(1 × C _B -(C)(C _E 1 × C-(H) ₃ (C))		
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	-54.90	- 60.42 106.66	5.52	75GOO/MES	Gas phase $\Delta_l H^\circ = C_p^\circ =$	56.40	55.83 136.74	0.57	90CHA/GAD
Liquid phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se - 95.10 181.21 241.04	- 93.65 189.23 237.88 - 604.71 86.64 - 34.95	- 1.45 - 8.02 3.16	75GOO/MES 81FIN/MES 81FIN/MES	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = 1 \text{ln} K_t =$	e -6.30 211.29	- 2.05 218.41 226.56 - 496.94 146.11 - 58.94	-4.25 -7.12	90CHA/GAD 1881REI
	$H_{2}(\mathbf{C})_{2}+(1)_{2}$ ohexane (su	.×C−(H)(C)₂(l b) rsc) e − Calculated		$C_6H_{13}N$ $H)_2(C)) +$ Reference		$(C_B)_2 + (C_B)_2 + (C_B)_1 + (C_B)_2 + (C_B)_1 + (C_B)_2 + (C_B$	(1 × C _B -(C)(C _B 1 × C-(H) ₃ (C)) re – Calculated	+(1×meta c	
Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 104.90	-100.99 134.60	-3.91	79STE	Gas phase $\Delta_t H^\circ = C_p^\circ =$	54.60	53.94 131.05	0.66	90CHA/GAD
Liquid phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se 147.70	- 145.03 216.76 238.71 - 740.19 75.66 - 30.52	-2.67	79STE	Liquid phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	-8.10 216.73	-5.31 214.91 226.56 -496.94 142.85 -57.63	- 2.79 1.82	90CHA/GAD 34KOL/UDO
Benzenami (5 × C _B -($(H)(C_B)_2) +$	(1×N-(H) ₂ (C _B e – Calculated		C_6H_7N $N)(C_B)_2), \sigma = 2$ Reference		$H)(C_B)_2) + H$ $H)(C_B)_2) + H$	$(1 \times C_B - (C)(C_B (1 \times N - (H)_2(C_B)))$))	
Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ - InK_t = S^\circ = S$	87.46 108.41 319.16	87.00 108.47 319.16 -268.03 166.91 -67.33	0.46 -0.06 0.00	90CHA/GAD 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ = C_t^\circ =$ $C_t^\circ =$ Liquid phase $\Delta_t H^\circ =$	55.30	54.57 130.34	0.73	90CHA/GAD
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	31.63 191.92 189.55	31.30 191.01 191.63 - 395.56 149.24 - 60.20	0.33 0.91 -2.08	90CHA/GAD 90CHA/GAD 90CHA/GAD	$ C_{\rho}^{r} = C_{\rho}^{r} = S^{\circ} - \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = $		-5.31 214.91 226.56 -496.94 142.85 -57.63		

N-Methylani (5 × C _B -(F (1 × C _B -(N	$I)(C_B)_2) + (1$	1×C-(H)₃(C))·	+ (1 × N-(H)	C_7H_9N (C)(C _B))+		$(C_B)_2$	Continued) (1×C _B -(N)(C ₁ ×-CH ₃ corr (c		$C_8H_{11}N$ $C)_2(C_B)) +$
	Literature	- Calculated =	Residual	Reference	·	Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_i H^\circ =$		84.49		····	Liquid phase $\Delta_t H^\circ = C_p^\circ =$	47.70 212.00	47.70 212.13	0.00 -0.13	82FUR/SAK 34KOL/UDO
Liquid phase $\Delta_t H^\circ = C_p^\circ =$	230.10	20.94 230.10	0.00	36KUR/VOS		$(C_B)_2 + ($	(1×C _B -(N)(C _I - (1×C-(H) ₃ (C		C _B H ₁₁ N H)(C)(C _B))+
Benzylamine (1 × N-(H		$\times C_{B}$ $-(H)(C_{B})_{2})$	+(1×C _B -(C	$(C_B)_2$ +		Literatur	e – Calculated	= Residual	Reference
		e – Calculated =	Residual	Reference	Gas phase $\Delta_i H^\circ =$	56.32	56.19	0.13	52VRI/HIL
Gas phase Δ _t H° =	87.80	87.80	0.00	77CAR/LAY	Liquid phase $\Delta_t H^\circ = C_p^\circ =$	4.02	- 9.86 260.52	13.88	52VRI/HIL
Liquid phase $\Delta_t H^\circ = C_p^\circ =$	e 34.20 207.19	34.20 205.88	0.00 1.31	77CAR/LAY 75NIC/WAD	N-Phenylanil (10×C _B -(1		(2×C _B -(N)(C	$(C_B)_2$) + $(1 \times N -$	C ₁₂ H ₁₁ N (H)(C _B) ₂)
2-Phenyleth	ylamine			C ₈ H ₁₁ N		Literature	e – Calculated	= Residual	Reference
	$C)(C_B)_2)+($	\times C-(H) ₂ (C)(N) 5 \times C _B -(H)(C _B) e – Calculated =	2)	1) ₂ (C)(C _B))+ Reference	Gas phase $\Delta_t H^\circ =$	219.30	219.05	0.25	53AIH
Gas phase $\Delta_t H^\circ =$		62.30		######################################	Liquid phase $\Delta_t H^\circ =$		135.10		
$C_p^* =$ Liquid phas $\Delta_t H^* =$	e	4.68			Solid phase $\Delta_l H^\circ = C_p^\circ =$	130.00	130.20 223.30	- 0.20	55MED
$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f = 0$	239.24	239.41 276.34 -583.47 178.64 -72.06	-0.17	75NIC/WAD	N-Methyl-N- (10 × C _B -(1 (1 × N-(C)	H)(C _B) ₂)+	ine (2×C _B -(N)(C	C _B) ₂) + (1 × C-	C13H13N (H)3(C))+
						Literatur	e – Calculated	= Residual	Reference
	$H)(C_B)_2) + ($	(1×C _B -(N)(C _B) ×-CH ₃ corr (qu		$C_8H_{11}N$ $C)_2(C_B)) +$	Gas phase $\Delta_t H^\circ =$		213.68		
	Literatur	e – Calculated =	Residual	Reference	Liquid phase				
Gas phase $\Delta_t H^\circ =$	100.50	100.51	-0.01	82FUR/SAK	$\Delta_i H^\circ = C_p^\circ =$	120.50 301.25	134.37 301.27	-13.87 -0.02	56TAV/LAM

(1 × NH ₂ -1		e – Calculated :	= Residual	Reference		Literature	Calculated	- Residual	Reference
					Gas phase				
Gas phase					$\Delta_{\rm f}H^{\circ} =$		91.14		
$\Delta_t H^\circ =$		91.14			$C_p^{\circ} =$		135.28		
$C_p^{\circ} =$		135.28							
					Liquid phase				
iquid phase	:				$\Delta_{\mathbf{f}}H^{\circ} =$		13.64		
$\Delta_{\rm f}H^{\circ} =$		13.64			$C_p^{\circ} =$		245.94		
$C_p^{\circ} =$		245.94			S° =		210.04		
S° =		210.04			Δ _f S° =		-538.18		
$\Delta_t S^\circ =$		-538.18			$\Delta_{\mathbf{f}}G^{\circ} =$		174.10		
$\Delta_{\rm f}G^{\circ} =$		174.10			$\ln K_{\rm f} =$		-70.23		
$\ln K_{\rm f} =$		-70.23					70.23		
					Solid phase				
Solid phase					$\Delta_{\rm f} H^{\circ} =$	6.40	2.42	3.98	73KUN/KAR
$\Delta_{\rm f}H^{\circ} =$	-0.30	-0.58	0.28	73KUN/KAR	$C_p^{\circ} =$		158.52		,02201,222
$C_p^{\circ} =$	0.50	158.52	0.20	752101 111	S° =		155.86		
$S^{\circ} =$		155.86			$\Delta_{\mathbf{f}}S^{\circ} =$		-592.36		
$\Delta_f S^\circ =$		-592.36			$\Delta_i G^{\circ} =$		179.03		
		176.03					- 72.22		
$\Delta_f G^\circ =$		1/0.03							
inK _f		-71.01			lnK _f	 	- 16.66		
1,3-Benzened		-71.01		C ₆ H ₈ N ₂	4-Aminobiph	$_{2}(C_{B})) + (1 \times$) ₂)+(9×C _B -(C ₁₂ H ₁₁
I,3-Benzened (4×C _B -(F		-71.01 (2×C _B -(N)(C _B) ₂) + (2×N–(1		4-Aminobiph	$_{2}(C_{B})) + (1 \times$) ₂)+(9×C _B -(
I,3-Benzened (4×C _B -(F	H)(C _B) ₂)+(NH ₂ meta	-71.01 (2×C _B -(N)(C _B			4-Aminobiph	$(C_B)_3$ + (1 × (C _B) ₃)		, , ,	
1,3-Benzened (4×C _B -(F	H)(C _B) ₂)+(NH ₂ meta	-71.01 $(2 \times C_{B} - (N)(C_{B} + (N))(C_{B} + (N))(C_{$		$(C_B) +$	4-Aminobiph (1×N-(H) + (2×C _B -($(C_B)_3$ + (1 × (C _B) ₃)	< С _в -(N)(С _в)	, , ,	H)(C _B) ₂)
1,3-Benzenec (4×C _B -(F (1×NH ₂)	H)(C _B) ₂)+(NH ₂ meta	-71.01 $(2 \times C_{B} - (N)(C_{B} + (N))(C_{B} + (N))(C_{$		$(C_B) +$	4-Aminobiph (1 × N-(H) + (2 × C _B -($(C_B)_3$ + (1 × (C _B) ₃)	← C _B −(N)(C _B)	, , ,	H)(C _B) ₂)
1,3-Benzenec (4×C _B -(F (1×NH ₂ -)	H)(C _B) ₂)+(NH ₂ meta	-71.01 (2×C _B -(N)(C _B corr) e - Calculated		$(C_B) +$	4-Aminobiph $(1 \times N - (H)) + (2 \times C_B - H)$ + (2 \times C_B - H) Gas phase $\Delta_t H^{\circ} =$	$(C_B)_3$ + (1 × (C _B) ₃)	C _B -(N)(C _B) - Calculated =	, , ,	H)(C _B) ₂)
1,3-Benzenec (4×C _B -(F (1×NH ₂ -)	H)(C _B) ₂)+(NH ₂ meta	-71.01 $(2 \times C_{B} - (N)(C_{B} + (N))(C_{B} + (N))(C_{$		$(C_B) +$	4-Aminobiph (1 × N-(H) + (2 × C _B -($(C_B)_3$ + (1 × (C _B) ₃)	← C _B −(N)(C _B)	, , ,	H)(C _B) ₂)
3-Benzeneck $(4 \times C_B - (F + (1 \times NH_2 - 1 \times NH_2 $	H)(C _B) ₂)+(NH ₂ meta	-71.01 (2 × C _B -(N)(C _B corr) e - Calculated		$(C_B) +$	4-Aminobiph $(1 \times N - (H)) + (2 \times C_B - H)$ + (2 \times C_B - H) Gas phase $\Delta_t H^{\circ} =$	$(C_B)_3$ + (1 × (C _B) ₃)	C _B -(N)(C _B) - Calculated =	, , ,	H)(C _B) ₂)
(4 × C _B -(F) (1 × NH ₂ -1) Gas phase $\Delta_t H^\circ = C_\rho^\circ =$	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2 × C _B -(N)(C _B corr) e - Calculated		$(C_B) +$	4-Aminobiph $(1 \times N - (H))$ $+ (2 \times C_B - (H))$ Gas phase $\Delta_t H^\circ = C_p^\circ = (H)$	$(C_B)_3$ + (1 × (C _B) ₃)	C _B -(N)(C _B) - Calculated =	, , ,	H)(C _B) ₂)
1,3-Benzenec $(4 \times C_B - (1 \times NH_2 - 1 \times N$	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2 × C _B -(N)(C _B corr) e - Calculated		$(C_B) +$	4-Aminobiph $(1 \times N - (H))$ $+ (2 \times C_B - H)$ $+ (2 \times C_B - H)$ Gas phase $\Delta_t H^\circ = C_p^\circ = $	$(C_B)_3$ + (1 × (C _B) ₃)	CC _B -(N)(C _B) - Calculated = 185.56 189.15	, , ,	H)(C _B) ₂)
Gas phase $C_{\rho}^{\alpha} = C_{\rho}^{\alpha} = C_{\rho}^$	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2×C _B -(N)(C _B corr) e - Calculated = 91.14 135.28		$(C_B) +$	4-Aminobiph $(1 \times N - (H))$ $+ (2 \times C_B - (H))$ Gas phase $\Delta_t H^\circ = C_p^\circ = C_p^$	$(C_B)_3$ + (1 × (C _B) ₃)	CC _B -(N)(C _B) - Calculated = 185.56 189.15	, , ,	H)(C _B) ₂)
Gas phase $C_{\rho}^{\alpha} = C_{\rho}^{\alpha} = C_{\rho}^$	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2×C _B -(N)(C _B corr) e - Calculated = 91.14 135.28		$(C_B) +$	4-Aminobiph $(1 \times N - (H))$ $+ (2 \times C_B - H)$ $+ (2 \times C_B - H)$ Gas phase $\Delta_t H^\circ = C_p^\circ = $	$(C_B)_3$ + (1 × (C _B) ₃)	CC _B -(N)(C _B) - Calculated = 185.56 189.15	, , ,	H)(C _B) ₂)
Gas phase $ \Delta_t H^\circ = C_p^\circ = C_p^\circ = S^\circ = S^\circ = C_p^\circ = C_p$	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2 × C _B -(N)(C _B corr) e - Calculated 91.14 135.28 13.64 245.94 210.04		$(C_B) +$	4-Aminobiph $(1 \times N - (H)) + (2 \times C_B - H)$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$	$(C_B)_3$ + (1 × (C _B) ₃)	CC _B -(N)(C _B) - Calculated = 185.56 189.15	, , ,	H)(C _B) ₂)
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = S^$	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2×C _B -(N)(C _B corr) e - Calculated = 91.14 135.28 13.64 245.94 210.04 -538.18		$(C_B) +$	4-Aminobiph $(1 \times N - (H)) + (2 \times C_B - H)$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ Solid phase	₂ (C _B)) + (1 × (C _B) ₃) Literature	C _B -(N)(C _B) - Calculated = 185.56 189.15 98.36 315.87	= Residual	H)(C _B) ₂) Reference
Gas phase $C_{\rho}^{\rho} = C_{\rho}^{\rho} = C_{\rho}^$	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2×C _B -(N)(C _B corr) e - Calculated = 91.14 135.28 13.64 245.94 210.04 -538.18 174.10		$(C_B) +$	4-Aminobiph $(1 \times N - (H)) + (2 \times C_B - H)$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = C_p^\circ =$	$(C_B)_3$ + (1 × (C _B) ₃)	C _B -(N)(C _B) - Calculated = 185.56 189.15 98.36 315.87	, , ,	H)(C _B) ₂)
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = S^$	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2 × C _B -(N)(C _B corr) e - Calculated 91.14 135.28 13.64 245.94 210.04 -538.18		$(C_B) +$	4-Aminobiph $(1 \times N - (H)) + (2 \times C_B - (H)) + (2 \times C_B - (H)) + (2 \times C_B - (H))$ Gas phase $\Delta_t H^\circ = C_p^\circ $	₂ (C _B)) + (1 × (C _B) ₃) Literature	185.56 189.15 98.36 315.87	= Residual	H)(C _B) ₂) Reference
Gas phase $C_{\rho}^{\rho} = C_{\rho}^{\rho} = C_{\rho}^$	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2×C _B -(N)(C _B corr) e - Calculated = 91.14 135.28 13.64 245.94 210.04 -538.18 174.10		$(C_B) +$	4-Aminobiph $(1 \times N - (H))$ $+ (2 \times C_{B^{-1}})$ Gas phase $\Delta_t H^{\circ} =$ $C_{\rho}^{\circ} =$ Liquid phase $\Delta_t H^{\circ} =$ $C_{\rho}^{\circ} =$ Solid phase $\Delta_t H^{\circ} =$ $C_{\rho}^{\circ} =$ $S^{\circ} =$	2(C _B)) + (1 × (C _B) ₃) Literature -	185.56 189.15 98.36 315.87 80.98 216.73 225.18	= Residual	H)(C _B) ₂) Reference
Gas phase $C_{p}^{A} = C_{p}^{A}$ $C_{p}^{A} = C_{p}^{A} = C_{p}^{A}$ $C_{p}^{A} = C_{p}^{A} = C_{p}^{A}$ $C_{p}^{A} = C_{p}^$	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2×C _B -(N)(C _B corr) e - Calculated = 91.14 135.28 13.64 245.94 210.04 -538.18 174.10		$(C_B) +$	4-Aminobiph $(1 \times N - (H))$ $+ (2 \times C_{B^{-1}})$ Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_p^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $\Delta_t S^\circ =$	2(C _B)) + (1 × (C _B) ₃) Literature -	185.56 189.15 98.36 315.87 80.98 216.73 225.18 -657.59	= Residual	H)(C _B) ₂) Reference
Gas phase $C_p^{\rho} = C_p^{\rho} = C_p^$	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2 × C _B -(N)(C _B corr) e - Calculated = 91.14 135.28 13.64 245.94 210.04 -538.18 174.10 -70.23	= Residual	H) ₂ (C _B)) + Reference	4-Aminobiph $(1 \times N - (H))$ $+ (2 \times C_{B^{-1}})$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	2(C _B)) + (1 × (C _B) ₃) Literature -	185.56 189.15 98.36 315.87 80.98 216.73 225.18 -657.59 277.04	= Residual	H)(C _B) ₂) Reference
Gas phase $C_{\rho}^{A} = C_{\rho}^{A}$ Gas phase $C_{\rho}^{A} = C_{\rho}^{A} = C_{\rho}^{A$	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2 × C _B -(N)(C _B corr) e - Calculated: 91.14 135.28 13.64 245.94 210.04 -538.18 174.10 -70.23	= Residual	H) ₂ (C _B)) + Reference 73KUN/KAR	4-Aminobiph $(1 \times N - (H))$ $+ (2 \times C_{B^{-1}})$ Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_p^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $\Delta_t S^\circ =$	2(C _B)) + (1 × (C _B) ₃) Literature -	185.56 189.15 98.36 315.87 80.98 216.73 225.18 -657.59	= Residual	H)(C _B) ₂) Reference
Gas phase $C_{\rho} = C_{\rho} = C_{\rho}$ Gas phase $C_{\rho} = C_{\rho} = C_{\rho}$ Solid phase $C_{\rho} = C_{\rho} = C_{\rho} = C_{\rho} = C_{\rho}$	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2 × C _B -(N)(C _B corr) e - Calculated: 91.14 135.28 13.64 245.94 210.04 -538.18 174.10 -70.23 -7.58 158.52	= Residual	H) ₂ (C _B)) + Reference	4-Aminobiph $(1 \times N - (H))$ $+ (2 \times C_{B^{-1}})$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	2(C _B)) + (1 × (C _B) ₃) Literature -	185.56 189.15 98.36 315.87 80.98 216.73 225.18 -657.59 277.04	= Residual	H)(C _B) ₂) Reference
Gas phase $ \begin{array}{l} (4 \times C_B - (1 \times NH_2 - 1)) \\ (1 \times NH_2 - 1) \end{array} $ Gas phase $ \begin{array}{l} \Delta_t H^\circ = \\ C_\rho^\circ = \\ \end{array} $ Liquid phase $ \begin{array}{l} \Delta_t H^\circ = \\ C_\rho^\circ = \\ \end{array} $ $ \begin{array}{l} \Delta_t S^\circ = \\ \Delta_t S^\circ = \\ \Delta_t G^\circ = \\ \end{array} $ Solid phase $ \begin{array}{l} \Delta_t H^\circ = \\ C_\rho^\circ = \\ S^\circ = \\ \end{array} $ Solid phase $ \begin{array}{l} \Delta_t H^\circ = \\ C_\rho^\circ = \\ S^\circ = \\ \end{array} $	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2 × C _B -(N)(C _B corr) e - Calculated = 91.14 135.28 13.64 245.94 210.04 -538.18 174.10 -70.23 -7.58 158.52 155.86	= Residual	H) ₂ (C _B)) + Reference 73KUN/KAR	4-Aminobiph $(1 \times N - (H))$ $+ (2 \times C_{B^{-1}})$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	2(C _B)) + (1 × (C _B) ₃) Literature -	185.56 189.15 98.36 315.87 80.98 216.73 225.18 -657.59 277.04	= Residual	H)(C _B) ₂) Reference
Gas phase $ \begin{array}{l} (4 \times C_B - (F + F)) \\ (1 \times NH_2 - F) \\ (1 \times NH_2 - F) \end{array} $ Gas phase $ \begin{array}{l} \Delta_t H^\circ = \\ C_p^\circ = \\ \end{array} $ Liquid phase $ \begin{array}{l} \Delta_t H^\circ = \\ C_p^\circ = \\ \end{array} $ $ \begin{array}{l} \Delta_t S^\circ = \\ \Delta_t G^\circ = \\ \end{array} $ in $K_t = $ Solid phase $ \begin{array}{l} \Delta_t H^\circ = \\ C_p^\circ = \\ S^\circ = \\ \Delta_t S^\circ = \\ \end{array} $ $ \begin{array}{l} \Delta_t S^\circ = \\ \Delta_t S^\circ = \\ \end{array} $	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2 × C _B -(N)(C _B corr) e - Calculated 91.14 135.28 13.64 245.94 210.04 -538.18 174.10 -70.23 -7.58 158.52 155.86 -592.36	= Residual	H) ₂ (C _B)) + Reference 73KUN/KAR	4-Aminobiph $(1 \times N - (H))$ $+ (2 \times C_{B^{-1}})$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	2(C _B)) + (1 × (C _B) ₃) Literature -	185.56 189.15 98.36 315.87 80.98 216.73 225.18 -657.59 277.04	= Residual	H)(C _B) ₂) Reference
Gas phase $ \begin{array}{l} (4 \times C_B - (1 \times NH_2 - 1)) \\ (1 \times NH_2 - 1) \end{array} $ Gas phase $ \begin{array}{l} \Delta_t H^\circ = \\ C_\rho^\circ = \\ \end{array} $ Liquid phase $ \begin{array}{l} \Delta_t H^\circ = \\ C_\rho^\circ = \\ \end{array} $ $ \begin{array}{l} \Delta_t S^\circ = \\ \Delta_t S^\circ = \\ \Delta_t G^\circ = \\ \end{array} $ Solid phase $ \begin{array}{l} \Delta_t H^\circ = \\ C_\rho^\circ = \\ S^\circ = \\ \end{array} $ Solid phase $ \begin{array}{l} \Delta_t H^\circ = \\ C_\rho^\circ = \\ S^\circ = \\ \end{array} $	H)(C _B) ₂) + (NH ₂ meta Literatur	-71.01 (2 × C _B -(N)(C _B corr) e - Calculated = 91.14 135.28 13.64 245.94 210.04 -538.18 174.10 -70.23 -7.58 158.52 155.86	= Residual	H) ₂ (C _B)) + Reference 73KUN/KAR	4-Aminobiph $(1 \times N - (H)) + (2 \times C_{B^{-1}}) + (2 \times C_{B^{-1}})$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ =$ $\Delta_t G^\circ =$	2(C _B)) + (1 × (C _B) ₃) Literature -	185.56 189.15 98.36 315.87 80.98 216.73 225.18 -657.59 277.04	= Residual	H)(C _B) ₂) Reference

TABLE 27. Imines (2)

TABLE 28. Nitriles (27)

	obutyleneim () ₃ (C)) + (2>	< C-(H)2(C)2) ·			Ethanenitri (1×C-(F	H)3(CN), A	cetonitrile), σ		C ₂ H ₃ I
	C))+(1×C _d corr (tertia	-(H)(C))+(1: ary))	< C-(H)(C)₂((C _d))+		Literatur	e – Calculated	= Residual	Reference
	Literature	e – Calculated	= Residual	Reference	Gas phase				
					$\Delta_t H^{\circ} =$	74.04	74.04	0.00	83AN/MAN
					$C_p^{\circ} =$	52.22	52.22	0.00	69STU/WES
Gas phase					<i>S</i> ° =	243.47	243.47	0.00	69STU/WES
$\Delta_{\rm f}H^{\circ} =$		- 84.71			$\Delta_f S^\circ =$		- 59.62		
					$\Delta_f G^\circ =$		91.82		
iouid Phos					$lnK_f =$		-37.04		
Liquid Phas Δ _ε H° =	– 132.80	- 129.74	-3.06	62BED/EDM					
					Liquid phas	se			
					$\Delta_t H^\circ =$	40.56	40.56	0.00	83AN/MAN
					$C_p^{\circ} =$	91.46	91.46	0.00	65PUT/MCE
N-(Phenylm	ethylene)be	nzenimine;			S° =	149.62	149.62	0.00	65PUT/MCE
	eneaniline			$C_{13}H_{11}N$	$\Delta_{\mathbf{f}}S^{\circ} =$		- 153.47		
$(10 \times C_B -$	$(H)(C_B)_2) +$	$(1 \times C_B - (N)) +$	$-(1 \times C_B - (C_d)$	$(C_B)_2) +$	$\Delta_l G^{\circ} =$		86.32		
		$1 \times N_{I} - (C_B)$			$lnK_f =$		-34.82		
	Literatur	e – Calculated	= Residual	Reference					· · · · · · · · · · · · · · · · · · ·
Can abasa					Propaneniti			NT\\ - 2	C ₃ H ₅ N
Gas phase $\Delta_t H^\circ =$	252.60	258.25	-4.65	48COA/SUT	(1×C-(F	1)3(C))+(1	\times C-(H) ₂ (C)(C	$N)), \sigma = 3$	
•	253.60	238.23 194.90	-4.03	48COA/SU1		T itamatuu	e - Calculated	Daaiduul	Reference
		194.90				Literatur	e – Calculated	= Residuai	Reference
$C_p^{\circ} =$									
					Gos aboss				
Liquid Phas	se	170.00			Gas phase	£1.50	50.04	0.54	TOLLOW THE P
Liquid Phas $\Delta_i H^\circ =$	se	178.90			$\Delta_t H^{\circ} =$	51.50	52.26	-0.76	
Liquid Phas $ \Delta_t H^\circ = C_p^\circ = $	se	302.68			$\Delta_t H^\circ = C_p^\circ =$	73.05	73.59	-0.54	69STU/WES
Liquid Phas $\Delta_t H^\circ = C_p^\circ = S^\circ =$	se	302.68 304.93			$\Delta_l H^\circ = C_p^\circ = S^\circ = C_p^\circ = C_p^$		73.59 285.44		
Liquid Phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$	se	302.68 304.93 -583.58			$\Delta_t H^\circ = C_p^\circ = S^\circ - \Delta_t S^\circ =$	73.05	73.59 285.44 -153.96	-0.54	69STU/WES
Liquid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S$	se	302.68 304.93 -583.58 352.89			$\Delta_t H^\circ = C_p^\circ = S^\circ - \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	73.05	73.59 285.44 -153.96 98.16	-0.54	69STU/WES
Liquid Phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$	se	302.68 304.93 -583.58			$\Delta_t H^\circ = C_p^\circ = S^\circ - \Delta_t S^\circ =$	73.05	73.59 285.44 -153.96	-0.54	69STU/WES
Liquid Phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $		302.68 304.93 -583.58 352.89			$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} - \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{f} = \frac{1}{2}$	73.05 286.60	73.59 285.44 -153.96 98.16	-0.54	69STU/WES
Liquid Phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = S$ Solid phase	·	302.68 304.93 - 583.58 352.89 - 142.36	_2.05	48COA/SUT	$\Delta_t H^\circ = C_p^\circ = S^\circ - \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ Liquid phas	73.05 286.60	73.59 285.44 -153.96 98.16 -39.60	-0.54 1.16	69STU/WES 69STU/WES
Liquid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S$		302.68 304.93 -583.58 352.89	- 2.05	48COA/SUT	$\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ \Delta_t S^\circ =$ $\ln K_f =$ Liquid phas $\Delta_t H^\circ =$	73.05 286.60	73.59 285.44 -153.96 98.16 -39.60	-0.54 1.16	69STU/WES 69STU/WES 71HAL/BAL
Liquid Phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = S$ Solid phase	·	302.68 304.93 - 583.58 352.89 - 142.36	-2.05	48COA/SUT	$\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ \Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ -$	73.05 286.60	73.59 285.44 -153.96 98.16 -39.60 18.46 119.49	-0.54 1.16 -2.96 0.01	69STU/WES 69STU/WES 71HAL/BAL 62WEB/KIL
Liquid Phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = S$ Solid phase	·	302.68 304.93 - 583.58 352.89 - 142.36	-2.05	48COA/SUT	$\Delta_t H^\circ =$ $C_\rho^\circ =$ $S^\circ \Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phas $\Delta_t H^\circ =$ $C_\rho^\circ S^\circ =$	73.05 286.60	73.59 285.44 -153.96 98.16 -39.60 18.46 119.49 189.32	-0.54 1.16	69STU/WES 69STU/WES 71HAL/BAL
Liquid Phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = S$ Solid phase	·	302.68 304.93 - 583.58 352.89 - 142.36	-2.05	48COA/SUT	$\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ \Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$	73.05 286.60	73.59 285.44 -153.96 98.16 -39.60 18.46 119.49 189.32 -250.08	-0.54 1.16 -2.96 0.01	69STU/WES 69STU/WES 71HAL/BAL 62WEB/KIL
Liquid Phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = S$ Solid phase	·	302.68 304.93 - 583.58 352.89 - 142.36	-2.05	48COA/SUT	$\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ \Delta_t S^\circ =$ $\ln K_t =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	73.05 286.60	73.59 285.44 -153.96 98.16 -39.60 18.46 119.49 189.32 -250.08 93.02	-0.54 1.16 -2.96 0.01	69STU/WES 71HAL/BAL 62WEB/KIL
Liquid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ Solid phase	·	302.68 304.93 - 583.58 352.89 - 142.36	-2.05	48COA/SUT	$\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ \Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$	73.05 286.60	73.59 285.44 -153.96 98.16 -39.60 18.46 119.49 189.32 -250.08	-0.54 1.16 -2.96 0.01	69STU/WES 69STU/WES 71HAL/BAL 62WEB/KIL
Liquid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = S$ Solid phase	·	302.68 304.93 - 583.58 352.89 - 142.36	-2.05	48COA/SUT	$\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ \Delta_t S^\circ =$ $\ln K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t -$ Butanenitrii	73.05 286.60	73.59 285.44 -153.96 98.16 -39.60 -39.60 -18.46 119.49 189.32 -250.08 93.02 -37.52	-0.54 1.16 -2.96 0.01 0.01	69STU/WES 69STU/WES 71HAL/BAL 62WEB/KIL 62WEB/KIL
Liquid Phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ Solid phase	·	302.68 304.93 - 583.58 352.89 - 142.36	-2.05	48COA/SUT	$\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ \Delta_t S^\circ =$ $\ln K_f =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t -$ Butanenitrii	73.05 286.60	73.59 285.44 -153.96 98.16 -39.60 -39.60 -18.46 119.49 189.32 -250.08 93.02 -37.52	-0.54 1.16 -2.96 0.01 0.01	69STU/WES 69STU/WES 71HAL/BAL 62WEB/KIL 62WEB/KIL

Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$

 $lnK_f =$

33.60

97.03 325.43

31.63

96.48 324.60

-251.11 106.50

-42.96

70HOW/WAD 69STU/WES 69STU/WES

1.97

0.55 0.83 TABLE 28. Nitriles (27) - Continued

TABLE 28. Nitriles (27) - Continued

	[)₃(C))+(1>	$(C-(H)_2(C)_2)$	sd) + (1 × C-(H) ₂ ($\begin{array}{c} C_4H_7N \\ (C)(CN)), \sigma = 3 \end{array}$	(1×C-(I	Octanenitrile; Capryonitrile $(1 \times C - (H)_3(C)) + (5 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2)$			
	Literature	- Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid phas	e								
$\Delta_{\mathbf{f}}H^{\circ} =$	- 5.82	-7.27	1.45	59EVA/SKI	Gas phase				
$C_{p}^{\circ} =$		149.91			$\Delta_{\rm f}H^{\circ} =$	-50.60	- 50.89	0.29	77STR/SUN
s° =		221.70			$C_p^{\circ} =$		188.04		
$\Delta_f S^\circ =$		-354.01			S° =		481.24		
$\Delta_f G^\circ =$		98.28			$\Delta_{6}S^{\circ} =$		-639.72		
$\ln K_f =$		- 39.64			$\Delta_f G^\circ =$		139.84		
			 		$lnK_f =$		-56.41		
Pentanenitr	ile; Valeron	itrile		C5H9N	Liquid pha	Se			
			+(1×C-/H)	$(C)(CN)$, $\sigma = 3$	$\Delta_t H^\circ =$	- 107.40	-110.19	2.79	77STR/SUN
(1 ^ C-(1)	1)3(C)) T (2)	· - (11/2(-/2)	· (1 ^ C-(11)2		$C_p^{\circ} =$	107.70	271.59	2.17	MOCATION
	T :44	Coloulated	– Davidual	Dafarana	S° =				
	Literature	- Calculated	= Residuai	Reference			351.22		
					$\Delta_{l}S^{\circ} =$		769.73		
					$\Delta_{\mathbf{f}}G^{\circ} =$		119.31		
Gas phase					$lnK_f =$		-48.13		
$\Delta_{\rm f}H^{\circ} =$	10.50	11.00	-0.50	70HOW/WAD					
$C_p^{\circ} =$		119.37							
S° =		363.76							
$\Delta_f S^{\circ} =$		-348.26			Decanenitri	ile; Capr i ni	itrile		C ₁₀ H ₁₉ N
$\Delta_{\mathbf{f}}G^{\circ} =$		114.83			(1×C-(H	(C) + (7)	×C-(H) ₂ (C) ₂)	+ (1 × C-(H))	$(C)(CN)), \sigma = 3$
$lnK_f =$		-46.32			((-		re – Calculated		Reference
						Littiatu		- Residual	Reference
Liquid phas	se								
$\Delta_f H^o =$	-33.10	-33.00	-0.10	69KON/PRO	Gas phase				
$C_{\rho}^{\circ} =$		180.33			$\Delta_t H^{\circ} =$	-91.60	-92.15	0.55	77STR/SUN
S° =		254.08			$C_{p}^{\circ} =$		233.82		
$\Delta_f S^\circ =$		- 457.94			S° =		559.56		
$\Delta_{\rm f}G^{\circ} =$		103.53			$\Delta_{f}S^{\circ} =$		-834.02		
$lnK_f =$		-41.77			$\Delta_{l}G^{\circ} =$		156,51		
			· · · · · · · · · · · · · · · · · · ·	1.000,000	$lnK_t =$		-63.14		
Heptaneniti	rile; Enanth		. (4 . 5 . (7)	C ₇ H ₁₃ N	Liquid phas				
(1 × C /T	1)3(C))+(4)	× U-(H)2(U)2)	+(1×C-(H)2	$(C)(CN)), \sigma = 3$	$\Delta_t H^\circ =$	- 158.40	- 161.65	3.25	77STR/SUN
$(1 \times C - (H$, , , , ,	· /- · /-/			1 2				
(1×C-(H					$C_p^{\circ} =$		332.43		
(1×C-(F		e – Calculated	= Residual	Reference	S° =		415.98		
(1 × C-(F			= Residual	Reference	$S^{\circ} = \Delta_{f}S^{\circ} =$		415.98 977.59		
			= Residual	Reference	$S^{\circ} = \Delta_{i}S^{\circ} = \Delta_{i}G^{\circ} = \Delta_{i}G^{\circ} = 0$		415.98		
(1 × C-(F	Literatur		= Residual	Reference	$S^{\circ} = \Delta_{f}S^{\circ} =$		415.98 977.59		
Gas phase $\Delta_t H^\circ =$			= Residual -0.74	Reference 73LEB/KAT	$S^{\circ} = \Delta_{i}S^{\circ} = \Delta_{i}G^{\circ} = \Delta_{i}G^{\circ} = 0$		415.98 977.59 129.82		
Gas phase	Literatur	e - Calculated			$S^{\circ} = \Delta_{i}S^{\circ} = \Delta_{i}G^{\circ} = \Delta_{i}G^{\circ} = 0$		415.98 977.59 129.82		
Gas phase $\Delta_t H^\circ =$	Literatur	e – Calculated – 30.26			$S^{\circ} = \Delta_{i}S^{\circ} = \Delta_{i}G^{\circ} = \Delta_{i}G^{\circ} = 0$		415.98 977.59 129.82		
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	Literatur	- 30.26 165.15 442.08			$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = -\infty$	itrile: Unde	415.98 - 977.59 129.82 - 52.37		CHN
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	Literatur	- 30.26 165.15 442.08 - 542.57			$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1}{2}$ Undecaneni		415.98 - 977.59 129.82 - 52.37	+ (1 × C-\H)·(C ₁₁ H ₂₁ N
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	Literatur	- 30.26 165.15 442.08 - 542.57 131.51			$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1}{2}$ Undecaneni		415.98 - 977.59 129.82 - 52.37	+ (1 × C-(H) ₂ ($C_{11}H_{21}N$ $C)(CN)), \sigma = 3$
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	Literatur	- 30.26 165.15 442.08 - 542.57			$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1}{2}$ Undecaneni	I) ₃ (C)) + (8	415.98 - 977.59 129.82 - 52.37		$C_{11}H_{21}N$ $C)(CN)), \sigma = 3$ Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	Literatur	- 30.26 165.15 442.08 - 542.57 131.51			$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1}{2}$ Undecaneni	I) ₃ (C)) + (8	415.98 - 977.59 129.82 - 52.37 ccylnitrile × C-(H) ₂ (C) ₂)		$C)(CN)), \sigma = 3$
Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f = $	Literatur	- 30.26 165.15 442.08 - 542.57 131.51		73LEB/KAT	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{2}$ Undecaneni	I) ₃ (C)) + (8	415.98 - 977.59 129.82 - 52.37 ccylnitrile × C-(H) ₂ (C) ₂)		$C)(CN)), \sigma = 3$
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = $ Liquid phas $\Delta_t H^\circ =$	Literatur – 31.00	- 30.26 165.15 442.08 - 542.57 131.51 - 53.05	-0.74		$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1}{1 \times C - (F)}$ Undecaneni (1 × C - (F)	I) ₃ (C)) + (8 Literatur	415.98 - 977.59 129.82 - 52.37 ccylnitrile × C-(H) ₂ (C) ₂)-	= Residual	C)(CN)), σ = 3 Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \ln K_t^\circ = Liquid phas \Delta_t H^\circ = C_p^\circ = 0$	Literatur – 31.00	-30.26 165.15 442.08 -542.57 131.51 -53.05	-0.74	73LEB/KAT	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{1 \times C - (F)}$ Undecaneni (1 × C - (F) Gas phase $\Delta_{t}H^{\circ} = \frac{1}{1 \times C - (F)}$	I) ₃ (C)) + (8	415.98 - 977.59 129.82 - 52.37 ccylnitrile × C-(H) ₂ (C) ₂)- re - Calculated		$C)(CN)), \sigma = 3$
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = S^\circ = $	Literatur – 31.00	-30.26 165.15 442.08 -542.57 131.51 -53.05 -84.46 241.17 318.84	-0.74	73LEB/KAT	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{1 \times C - (H)}$ Undecaneni (1 × C - (H)) Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = \frac{1}{1 \times C}$	I) ₃ (C)) + (8 Literatur	415.98 - 977.59 129.82 - 52.37 ecylnitrile × C-(H) ₂ (C) ₂) re - Calculated - 112.78 256.71	= Residual	C)(CN)), σ = 3 Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t$	Literatur – 31.00	-30.26 165.15 442.08 -542.57 131.51 -53.05 -84.46 241.17 318.84 -665.80	-0.74	73LEB/KAT	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{1 \times C - (H)}$ Undecaneni (1 × C - (H) Gas phase $\Delta_{t}H^{\circ} = C_{r}^{\circ} = S^{\circ} = \frac{1}{1 \times C - (H)}$	I) ₃ (C)) + (8 Literatur	415.98 - 977.59 129.82 - 52.37 ccylnitrile × C-(H) ₂ (C) ₂) re - Calculated -112.78 256.71 598.72	= Residual	C)(CN)), σ = 3 Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t$	Literatur – 31.00	-30.26 165.15 442.08 -542.57 131.51 -53.05 -84.46 241.17 318.84 -665.80 114.05	-0.74	73LEB/KAT	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{1}$ Undecaneni (1 × C-(H) Gas phase $\Delta_{t}H^{\circ} = C_{r}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \frac{1}{1}$	I) ₃ (C)) + (8 Literatur	415.98 - 977.59 129.82 - 52.37 cylnitrile × C-(H) ₂ (C) ₂) re - Calculated - 112.78 256.71 598.72 - 931.17	= Residual	C)(CN)), σ = 3 Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t$	Literatur – 31.00	-30.26 165.15 442.08 -542.57 131.51 -53.05 -84.46 241.17 318.84 -665.80	-0.74	73LEB/KAT	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{1}{1 \times C - (H)}$ Undecaneni (1 × C - (H) Gas phase $\Delta_{t}H^{\circ} = C_{r}^{\circ} = S^{\circ} = \frac{1}{1 \times C - (H)}$	I) ₃ (C)) + (8 Literatur	415.98 - 977.59 129.82 - 52.37 ccylnitrile × C-(H) ₂ (C) ₂) re - Calculated -112.78 256.71 598.72	= Residual	C)(CN)), σ = 3 Reference

TABLE 28.	Nitriles	(27) –	Continued
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TABLE 2	28. Nii	triles ((27)	- (Continued
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	Literatur	e – Calculated =	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Liquid phas	e e				***				
$\Delta_{i}H^{\circ} =$		-187.38	2.88	77STR/SUN	Gas phase				
$C_p^{\circ} =$	'	362.85			$\Delta_i H^{\circ} =$	140.71	140.71	0.00	73KON
S° =		448.36			$C_p^o =$		86.85	****	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
$\Delta_i S^\circ =$		- 1081.53			~ <i>p</i>		00.00		
$\Delta_{f}G^{\circ} =$		135.08							
$\ln K_{\rm f} =$		- 54.49			Liquid phas	e			*
IIIV!		-34.43			$\Delta_{\rm f}H^{\circ} =$	100.71	100.72	-0.01	60VON/DDO
					$C_p^{\circ} =$	100.71	141.50	-0.01	69KON/PRO
					$S^{\circ} =$		204.60		
T-4 3	idadlaa D#s			CHN	$\Delta_{t}S^{\circ} =$				
		ristonitrile		C ₁₄ H ₂₇ N			- 240.54		
(1×C-(F	1)₃(C))+(1	$1 \times C - (H)_2(C)_2$)+(1×C-(H)	$_2(C)(CN)), \sigma = 3$	$\Delta_t G^{\circ} =$		172.44		
	T itamatu	re – Calculated:	– Doridual	Reference	$lnK_f =$		-69.56		
	Lateratu	re – Calculateu	= Kesiduai	Reference					
Gas phase					cis -2-Butene	nitrile			C ₄ H ₅ N
$\Delta_t H^{\circ} =$	-174.80	-174.67	-0.13	77STR/SUN	(1×C-(H	() ₃ (C)) + (1	$\times C_d$ -(H)(C))	$+(1\times C_{d}-(H)($	CN))+
$C_p^{\circ} =$		325.38			$(1 \times cis)$	nsat) corr)			
S° =		716.20							
$\Delta_f S^{\circ} =$		-1222.62				Literatur	e – Calculated	= Residual	Reference
$\Delta_l G^{\circ} -$		189.86							
$lnK_{f} =$		- 76.59							
•					Gas phase				
					$\Delta_f H^{\circ} =$	134.10	145.56	- 11.46	73KON
Liquid pha	se				$C_p^{\circ} =$		78.82		
$\Delta_t H^\circ =$	- 260.10	-264.57	4.47	77STR/SUN					
$C_p^{\circ} =$	200.10	454.11		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,					
$S^{\circ} =$		545.50			Liquid phas	e			
$\Delta_{\rm f}S^{\circ} =$		- 1393.32			$\Delta_{\rm f}H^{\circ} =$	95.10	105.99	- 10.89	69KON/PRO
		150.85				25.10	141.50	- 10.07	OJKONI KO
$\Delta_f G^{\circ} =$					$C_p^{\circ} = S^{\circ} =$				
$lnK_{f} =$		- 60.85					204.60		
					$\Delta_{\mathbf{f}}S^{\circ} =$		-240.54		
					$\Delta_i G^{\circ} -$		177.71		
				C ₃ H ₃ N	$lnK_f =$		-71.69		
				I HAN					
		nitrile C _d -(H)(CN)), o	r = 1	Callan					
	$(H)_2) + (1 \times$			Reference	2-Methylpro	panenitrile	; Isobutryonit	rile	C₄H ₇ N
	$(H)_2) + (1 \times$	C _d -(H)(CN)), o			(2×C-(H	() ₃ (C))+(1	\times C-(H)(C) ₂ (0		C₄H ₇ N
	(H) ₂) + (1 ×	C _d -(H)(CN)), o			(2×C-(H		\times C-(H)(C) ₂ (0		C₄H ₇ N
(1×C _d -((H) ₂) + (1 ×	C _d -(H)(CN)), o	= Residual		(2×C-(H	i) ₃ (C)) + (1: corr (tertia	\times C-(H)(C) ₂ (0	CN))+	C₄H ₇ N Reference
$(1 \times C_{d} - (1 $	(H) ₂) + (1 × Literatu	C _d -(H)(CN)), our e - Calculated	= Residual	Reference	(2×C-(H	i) ₃ (C)) + (1: corr (tertia	× C-(H)(C) ₂ (C ary))	CN))+	
$(1 \times C_{d} - (1 $	(H) ₂) + (1 × Literatu 183.68 64.18	C _d -(H)(CN)), our e - Calculated 172.97 63.76	= Residual 10.71 0.42	Reference 72FIN/MES 72FIN/MES	(2×C-(H	i) ₃ (C)) + (1: corr (tertia	× C-(H)(C) ₂ (C ary))	CN))+	
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	(H) ₂) + (1 × Literatu	C _d -(H)(CN)), our e - Calculated 172.97 63.76 273.93	= Residual	Reference 72FIN/MES	(2×C-(H (2×-CH₃	i) ₃ (C)) + (1: corr (tertia	× C-(H)(C) ₂ (C ary))	CN))+	
Gas phase $ \Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = S^\circ$	(H) ₂) + (1 × Literatu 183.68 64.18	C _d -(H)(CN)), our e - Calculated 172.97 63.76 273.93 - 34.90	= Residual 10.71 0.42	Reference 72FIN/MES 72FIN/MES	(2×C-(H (2×-CH ₃	Literatur	× C-(H)(C) ₂ (C ary)) e – Calculated	CN)) + = Residual	Reference
Gas phase $\Delta_i H^\circ = C_p^\circ = S^\circ =$	(H) ₂) + (1 × Literatu 183.68 64.18	C _d -(H)(CN)), our e - Calculated 172.97 63.76 273.93	= Residual 10.71 0.42	Reference 72FIN/MES 72FIN/MES	(2×C-(H (2×-CH₃	i) ₃ (C)) + (1: corr (tertia	× C-(H)(C) ₂ (C ary))	CN))+	, ,
Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \ln K_f = \frac{1}{2}$	183.68 64.18 275.31	172.97 63.76 273.93 - 34.90 183.37	= Residual 10.71 0.42	Reference 72FIN/MES 72FIN/MES	$(2 \times C - (H_3))$ $(2 \times -CH_3)$ $Cas phase$ $\Delta_l H^o = C_p^o =$	(2) ₃ (C)) + (1) ₃ (C)) + (1) ₃ (C) + (1) ₄ (C) + (1)	× C-(H)(C) ₂ ((ary)) e - Calculated 24.46	CN)) + = Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_f = $ Liquid pha	183.68 64.18 275.31	172.97 63.76 273.93 - 34.90 183.37 - 73.97	10.71 0.42 1.38	72FIN/MES 72FIN/MES 72FIN/MES	$(2 \times C - (H + (2 \times -CH_3))^2 + (2 \times -CH_3)^2$ Gas phase $\Delta_t H^\circ = C_p^\circ = C$	(2)(C)) + (1)(C)) + (1)(C) Corr (tertial Literatur 23.30	× C-(H)(C)₂(Cary)) e - Calculated 24.46 96.40	= Residual = 1.16	Reference 70HOW/WAD
Gas phase $\Delta_t H^\circ = C_\rho^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = -\frac{\Delta_t H^\circ}{\Delta_t H^\circ} = \frac{\Delta_t H^\circ}{\Delta_t H^\circ} = \Delta_t H$	183.68 64.18 275.31	172.97 63.76 273.93 - 34.90 183.37 - 73.97	10.71 0.42 1.38	Reference 72FIN/MES 72FIN/MES 72FIN/MES	$(2 \times C - (H + (2 \times -CH_3)))$ $Cas phase$ $\Delta_l H^\circ = C_p^\circ = $	23.30 e - 13.80	× C-(H)(C) ₂ (Gary)) e - Calculated 24.46 96.40 - 18.08	= Residual -1.16	Reference 70HOW/WAD 71HAL/BAL
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{\Delta_t H^\circ}{\Delta_t H^\circ} = C_p^\circ = C_p^\circ = C_p^\circ = \frac{\Delta_t H^\circ}{\Delta_t H^\circ} = \frac{\Delta_t H^\circ}{\Delta_t$	183.68 64.18 275.31	172.97 63.76 273.93 - 34.90 183.37 - 73.97	10.71 0.42 1.38	72FIN/MES 72FIN/MES 72FIN/MES	$(2 \times C - (H + (2 \times -CH_3))^2 + (2 \times -CH_3)^2$ Gas phase $\Delta_t H^\circ = C_p^\circ = C$	(2)(C)) + (1)(C)) + (1)(C) Corr (tertial Literatur 23.30	× C-(H)(C)₂(Cary)) e - Calculated 24.46 96.40	= Residual = 1.16	Reference 70HOW/WAD
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \frac{\Delta_{t}H^{\circ}}{\Delta_{t}H^{\circ}} = C_{p}^{\circ} = S^{\circ} = S^{\circ} = \frac{\Delta_{t}H^{\circ}}{S^{\circ}} = \frac{\Delta_{t}H^{\circ}}$	183.68 64.18 275.31	172.97 63.76 273.93 - 34.90 183.37 - 73.97	10.71 0.42 1.38	Reference 72FIN/MES 72FIN/MES 72FIN/MES	$(2 \times C - (H + (2 \times -CH_3)))$ $Cas phase$ $\Delta_l H^\circ = C_p^\circ = $	23.30 e - 13.80	× C-(H)(C) ₂ (Gary)) e - Calculated 24.46 96.40 - 18.08	= Residual -1.16	Reference 70HOW/WAD 71HAL/BAL
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \frac{\Delta_t H^\circ}{\Delta_t H^\circ} = C_p^\circ = C_p^\circ = C_p^\circ = \frac{\Delta_t H^\circ}{\Delta_t H^\circ} = \frac{\Delta_t H^\circ}{\Delta_t$	183.68 64.18 275.31	172.97 63.76 273.93 - 34.90 183.37 - 73.97	10.71 0.42 1.38	Reference 72FIN/MES 72FIN/MES 72FIN/MES 72FIN/MES 72FIN/MES	$(2 \times C - (H + (2 \times -CH_3)))$ $Cas phase$ $\Delta_l H^\circ = C_p^\circ = $	23.30 e - 13.80	× C-(H)(C) ₂ (Gary)) e - Calculated 24.46 96.40 - 18.08	= Residual -1.16	Reference 70HOW/WAD 71HAL/BAL
Gas phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \ln K_f = \frac{\Delta_t H^{\circ}}{\Delta_t H^{\circ}} = \frac{\Delta_t H^{\circ}}{\Delta_t H^{\circ}} = \frac{\Delta_t H^{\circ}}{S^{\circ}} = \frac{\Delta_t H^{\circ}}{S^{\circ}$	183.68 64.18 275.31	172.97 63.76 273.93 - 34.90 183.37 - 73.97	10.71 0.42 1.38	Reference 72FIN/MES 72FIN/MES 72FIN/MES 72FIN/MES 72FIN/MES	$(2 \times C - (H + (2 \times -CH_3)))$ $Cas phase$ $\Delta_l H^\circ = C_p^\circ = $	23.30 e - 13.80	× C-(H)(C) ₂ (Gary)) e - Calculated 24.46 96.40 - 18.08	= Residual -1.16	Reference 70HOW/WAD 71HAL/BAL

TABLE 28. Nitriles (27) - Continued

TABLE 28. Nitriles (27) - Continued

trans - 2 - Pento (1 × C - (H) (1 × C _d - (H)) ₃ (C))+(1>	< C-(H) ₂ (C)(C _c	i)) + (1 × C _d -(C_5H_7N $(H)(C)) +$			×C-(H)(C)2(C ile rsc)	CN))+	C ₄ H ₅ N
	Literature	e – Calculated =	= Residual	Reference	* W## * * * * * * * * * * * * * * * * *	Literatur	e – Calculated =	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	119.79	119.83 107.48	-0.04	73KON	Gas phase Δ _I H° =	182.80	182.80	0.00	82FUC/HAL
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	e 74.89	74.99 170.79 236.27	-0.10	69KON/PRO	Liquid phas $\Delta_t H^\circ = C_p^\circ =$	140.80 115.40	140.80 115.40	0.00	71HAL/BAL 71HAL/BAL
$\Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = -1$		-345.18 177.90 -71.77					× C-(H)(C) ₂ (C e rsc)	CN))+	C ₅ H ₇ N
trans -3-Pent	enenitrile			C₅H₂N		Literatur	e – Calculated =	= Residual	Reference
		× C _d -(H)(C)) +	$(1 \times C - (H)_2)$		a				
	Literatur	e – Calculated =	= Residual	Reference	Gas phase $\Delta_t H^\circ =$	143.00	143.00	0.00	71HAL/BAL
Gas phase $\Delta_t H^\circ =$	125.69	125.69	0.00	73KON	Liquid phas $\Delta_t H^\circ = C_p^\circ =$	e 103.00 146.00	103.00 146.00	0.00	71HAL/BAL 71HAL/BAL
Liquid phas $\Delta_t H^\circ =$	80.88	80.89	-0.01	69KON/PRO	Cyclopentar	nenitrile			C ₆ H ₉ N
		\times C-(C) ₃ (CN))	+	C₅H ₉ N		pentanenitr	× C-(H)(C)z(C ile rsc) e - Calculated =		Reference
	Literatur	e – Calculated	= Residual	Reference	Gas phase $\Delta_t H^\circ =$	41.80	41.80	0.00	71HAL/BAL
Gas phase $\Delta_t H^\circ =$	- 2.50	-2.50	0.00	70HOW/WAD	Liquid phas				
Liquid phas					$\Delta_l H^0 = C_p^\circ =$	0.70 167.50	0.70 167.50	0.00	71HAL/BAL 71HAL/BAL
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = $	-39.80 179.37 232.00	- 39.80 179.35 231.99 - 480.03 103.32	0.00 0.02 0.01	71HAL/BAL 67WES/RIB 67WFS/RIB		enitrile l) ₂ (C) ₂) + (1 hexanenitril	×C-(H)(C)2(C e rsc)	:N))+	C7H11N
$lnK_f =$		-41.68		·		Literatur	e – Calculated -	- Residual	Reference
					Gas phase $\Delta_t H^\circ =$	4.80	4.80	0.00	71HAL/BAL
					Liquid phas $\Delta_t H^\circ = C_p^\circ =$	e -47.20 177.90	-47.20 177.90	0.00 0.00	71HAL/BAL 71HAL/BAL

TABLE 28. Nitriles (27) - Continued

TABLE 27. Nitriles (27) - Continued

Benzonitrile (5×C _B -(H	$)(C_B)_2)+($	1×C _B -(CN)(C	$(C_{\rm B})_2$), $\sigma = 2$	C ₇ H ₅ N	1,5-Pentane (1×C-(H		lutaronitrile !×C-(H) ₂ (C)(CN))	C ₅ H ₆ N ₂	
	Literature	- Calculated	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference	
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	218.82 109.08 321.04	220.05 109.14 321.04	-1.23 -0.06 0.00	59EVA/SKI 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ =$		168.41 118.61			
$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	<u>.</u>	-141.32 262.18 -105.76	and the state of t		Liquid phase $\Delta_l H^\circ = C_p^\circ =$	e 186.26	106.41 196.44	- 10.18	65CLE/WUL	
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	163.18 165.20 209.10	163.18 165.20 209.10	0.00 0.00 0.00	59EVA/SKI 84LEB/BYK 84LEB/BYK	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = -\infty$	239.45	244.42 -367.49 215.98 -87.12	- 4.97 	65CLE/WUL	
$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		- 253.26 238.69 - 96.29			Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	102.90	110.29 167.52 215.31	-7.39	1889BER/PE	
2-Butyne-1,4 (2×C₁–(C				C ₄ N ₂	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		- 396.60 228.54 - 92.19			
	Literatur	e – Calculated	= Residual	Reference					•	
Gas phase Δ _t H° =	529.28	529.20	0.08	57SAG			× C-(C)₂(CN);	2)+	C₅H₄N	
Liquid phase Δ _t H° =	500.41	500.40	0.01	63ARM/MAR		erature-Cal	culated = Resid	dual Refere	nce	
1,4-Butaned	initrile; Su)2(C)(CN)			C ₄ H ₄ N ₂	Solid phase $C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} =$	179.49 187.95	179.50 187.95 -423.96	0.01 0.00	67RIB/WES 67RIB/WES	
	, ,	re – Calculated	= Residual	Reference	1,6-Hexaned		•		C₅H₅N	
Gas phase $\Delta_t H^\circ = C_p^\circ =$	209.70	189.04 95.72	20.66	71RAP/WES	(2×C-(H		e – Calculated	**	Reference	
Liquid phase $\Delta_l H^\circ = C_p^\circ =$	e	132.14 166.02			Gas phase $\Delta_t H^\circ = C_p^\circ =$	149.50	147.78 141.50	1.72	73LEB/KAT	
$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$		212.04 - 263.56 210.72 - 85.00			Liquid phase $ \Delta_t H^\circ = \\ C_\rho^\circ = \\ S^\circ = $	e 85.10	80.68 226.86 276.80	4.42	73LEB/KAT	
Solid phase $\Delta_l H^\circ = C_p^\circ = S^\circ =$	139.70 145.60 191.59	139.70 145.60 192.30	0.00 0.00 - 0.71	71RAP/WES 63WUL/WES 63WUL/WES	$\Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = -\frac{1}{2}$		- 471.42 221.24 - 89.24			
$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-283.30 224.17 -90.43	2							

TABLE 28. Nitriles (27) - Continued

TABLE 29. Hydrazi	nes (6)
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	TABLE	28. Nitriles (2	7) – Continu	ied			FABLE 29. Hydi	razines (6)	
		Dicyanobenzen (2×C _B -(CN)(C ₈ H ₄ N ₂	Hydrazine (2×N-(H		N₂H₄		
	Literatu	re – Calculated	= Residual	Reference		Literature - Calculated = Residual			Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	358.30	357.24 136.62	1.06	92ACR/TUC	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = 0$	95.19 52.71 238.36	95.40 52.72 238.60	-0.21 -0.01 -0.24	49SCO/OLI 49SCO/OLI 49SCO/OLI
Liquid phase $\Delta_t H^\circ = C_p^\circ =$	e	277.40 194.32			$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-214.05 159.22 -64.23		
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1}{2}$ Solid phase $\Delta_t H^{\circ} = \frac{1}{2}$	268.50	244.98 - 253.58 353.01 - 142.40 268.52	-0.02	92ACR/TUC	Liquid phase $\Delta_t H^\circ = C_\theta^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	50.42 98.83 121.21	50.60 98.82 121.16 -331.48 149.43 -60.28	-0.18 0.01 0.05	39HUG/COR 49SCO/OLI 49SCO/OLI
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = -\frac{1}{2}$		191.90 - 306.66 359.95 - 145.20			Methylhydra (1×C-(H		×N-(H)(C)(N)))+(1×N-(H	CH ₆ N ₂
						Literatur	e – Calculated =	= Residual	Reference
					Gas phase $\Delta_t H^\circ =$	94.60	94.60	0.00	51AST/FIN
					Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	54.20 134.93 165.94	52.69 134.93 165.93 - 423.02 178.81 - 72.13	1.51 0.00 0.01	51AST/ROC 51AST/FIN 51AST/FIN
	·				1,1-Dimethyl (2×C-(H)	hydrazine) ₃ (N))+(1	× N-(C)2(N))+	(1×N−(H) ₂ (C ₂ H ₈ N ₂ N))
						Literatur	e – Calculated =	= Residual	Reference
					Gas phase $\Delta_t H^\circ =$	83.89	83.89	0.00	53AST/WOO
					Liquid phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	49.30 164.05 200.25	49.08 164.04 200.24 - 525.02 205.62 - 82.94	0.22 0.01 0.01	60DON/SHO 53AST/WOO 53AST/WOO

 $C_2H_8N_2\\$

Reference

51AST/JAN

52AST/ROC

Reference

72LEB/KAT

72LEB/KAT

11LOU/DUP

Reference

51COL/GIL

 $C_{12}H_{12}N_2$

 $C_6H_8N_2$

1,2-Dimethylhydrazine

Gas phase

Liquid phase $\Delta_{i}H^{\circ} = C_{p}^{\circ} = S^{\circ} =$

 $\Delta_f S^\circ =$

 $\Delta_{\rm f}G^{\circ} =$

 $lnK_f =$

Gas phase $\Delta_i H^\circ =$

Liquid phase

Solid phase

Gas phase $\Delta_t H^\circ =$

Liquid phase $\Delta_i H^\circ =$

Solid phase $\Delta_t H^{\circ} =$

 $\Delta_{\rm f}H^{\circ} =$

 $\Delta_{\rm f}H^{\circ} =$

Phenylhydrazine

 $(1 \times N - (H)_2(N))$

202.90

141.00

124.60

221.30

1,2-Diphenylhydrazine; Hydrazobenzene

 $\Delta_t H^\circ =$

 $(2 \times C - (H)_3(N)) + (2 \times N - (H)(C)(N))$

92.01

52.70

TABLE	29.	Hydrazines	(6)	_	Continued
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Literature - Calculated = Residual

93.80

54.78

171.04 210.70

-514.56

208.20

-83.99

 $(5 \times C_B - (H)(C_B)_2) + (1 \times C_B - (N)(C_B)_2) + (1 \times N - (H)(C_B)(N)) +$

Literature-Calculated=Residual

202.95

141.00

128.27

 $(10 \times C_B - (H)(C_B)_2) + (2 \times C_B - (N)(C_B)_2) + (2 \times N - (H)(C_B)(N))$ Literature-Calculated=Residual

310.50

231.40

218.60

-1.79

-2.08

-0.05

0.00

-3.67

2.70

Dimethyldiaz (2×C-(H)		ethane 2×N _A –(C))		C ₂ H ₆ l
	Literatur	e – Calculated	= Residual	Reference
Gas phase Δ _i H° =	134.47	134.48	- 0.01	76ROS
	$_{3}(C)) + (13)$	ethyl azoethan × C-(H) ₂ (C)(A		C ₃ H ₈ l -(C)) +
	Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_l H^\circ =$	113.85	113.78	0.07.	76ROS
Diethyldiazei (2×C-(H)		ane × C–(H) ₂ (C)(Λ	/ _A))+(2× <i>N</i> _A -	C4H101 (C))
	Literature	e – Calculated	= Residual	Reference
Gas phase Δ _I H° =	93.26	93.08	0.18	76ROS
				
Di-n-propyld (2×C-(H) (2×N _A -(C	3(C))+(2)	opropane < C-(H) ₂ (C) ₂)	+ (2×C-(H) ₂ (
(2×C-(H)	(2) (2) (3) (3) (4)			
(2×C-(H)	(2) (2) (3) (3) (4)	C-(H) ₂ (C) ₂		C)(N _A)) + Reference
(2×C-(H) (2×N _A -(C)	(3(C)) + (2×2)) Literature 51.34	C-(H) ₂ (C) ₂	= Residual	C)(N _A)) + Reference
$(2 \times C - (H))$ $(2 \times N_A - (C))$ Gas phase $\Delta_t H^{\circ} =$ Liquid phase $\Delta_t H^{\circ} =$ Methyl-n-but $(1 \times C - (H))$	(2) (2) (2) (2) (3) (2) (3) (2) (4) (4) (4) (4) (4) (4) (4) (4) (4) (4	C-(H) ₂ (C) ₂ = - Calculated 51.82	= Residual -0.48	C)(N _A)) + Reference 76ENG/MEL 76ENG/MEL C ₈ H ₁₂ I
$(2 \times C - (H))$ $(2 \times N_A - (C))$ Gas phase $\Delta_t H^{\circ} =$ Liquid phase $\Delta_t H^{\circ} =$ Methyl-n-but $(1 \times C - (H))$	(2) + (2) (2)) Literature 51.34 11.50 (y)diazene (3)(C)) + (2) (2)) + (1 × C	51.82 11.62	= Residual -0.48 -0.12 + (1 × C-(H) ₂ (C)(N _A)) + Reference 76ENG/MEL 76ENG/MEL C ₈ H ₁₂ I
$(2 \times C - (H))$ $(2 \times N_A - (C))$ Gas phase $\Delta_t H^{\circ} =$ Liquid phase $\Delta_t H^{\circ} =$ Methyl-n-but $(1 \times C - (H))$	(2) + (2) (2)) Literature 51.34 11.50 (y)diazene (3)(C)) + (2) (2)) + (1 × C	51.82 11.62 CC-(H) ₂ (C) ₂) (C-(H) ₂ (C) ₂) (H) ₃ (N _A))	= Residual -0.48 -0.12 + (1 × C-(H) ₂ (Reference 76ENG/MEL 76ENG/MEL C ₅ H ₁₂ N C)(N _A)) +

TABLE 30.	Diazenes	(14) -	Continued
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TABLE 30. Diazenes (14) - Continued

(4×C-(H) ₃ (C)) + (4	oisopropane ×-CH ₃ corr (to +(2×N _A -(C))	ertiary))+	C ₆ H ₁₄ N ₂	(10×C-	$(H)_3(C)) + ($	butyl)diazene 2×N _A -(C))+(: at/quat))+(2×		$C_{16}H_{34}N_2$ $(2 \times C - (C)_4) +$
	Literatur	e – Calculated :	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase Δ _t H° =	35.60	35.60	0.00	76ENG/MEL	Gas phase Δ _t H° =	- 196.80	-189.86	- 6.94	76ENG/MEL
Liquid phase Δ _t H° =	e -0.30	-0.30	0.00	76ENG/MEL	Liquid pha $\Delta_t H^\circ =$	ase - 263.30	-257.28	- 6.02	76ENG/MEL
Di-n -butyldi (2×C–(H (2×N _A –() ₃ (C)) + (4	butane × C–(H)2(C)2) -	+ (2×C−(H) ₂ ($C_8H_{18}N_2$ $(C)(N_A)) +$	Tetrame	thyl-1-pyraz			C7H14N2
	Literatur	e – Calculated :	= Residual	Reference	(4×-CH	+ I ₃ corr (quai	!/quat))+	2× <i>N</i> _A (C))+	$(2 \times C - (C)_3(N_A))$
Gas phase Δ _f H° =	9.20	10.56	-1.36	78ENG/MON	(1 × Cyc	•	nediazene rsc) re – Calculated:	= Residual	Reference
Liquid phas Δ _t H° =	e -40.10	- 39.84	-0.26	78ENG/MON	Gas phase Δ _t H° =	39.30	39.30	0.00	76ENG/MEL
(6×C-(H	(3)(C) + (2)	zo-tert-butane \times C-(C) ₃ (N_A)) ternary)) + (2 \times		C ₈ H ₁₈ N ₂	Solid phase $\Delta_t H^\circ =$	e -22.30	- 22.30	0.00	76ENG/MEL
(011-011)	`•	re – Calculated		Reference			otetramethylen etramethyl-pyric		,
Gas phase Δ _t H° =	-35.61	-38.92	3.31	76ENG/MEL	$(4 \times C - (1 \times N_A - $	H) ₃ (C))+(4 (C))+(2×0		uat/quat))+($C_8H_{16}N_2$ 2×C-(H) ₂ (C) ₂)+
Liquid phas		71.20	2.40	TCENCA (EL	•	Literatui	e – Calculated =	= Residual	Reference
Δ _f H° =	74.70 	-71.30	-3.40	76ENG/MEL	Gas phase $\Delta_t H^\circ =$	42.00	42.00	0.00	76ENG/MEL
(8×C-(H (3×-CH ₃	$()_3(C)) + (2$	$(2 \times (2 \times$	× C-(H) ₂ (C) ₂	$C_{12}H_{26}N_2$ + (1 × C-(C) ₄) +	Liquid pha $\Delta_t H^\circ =$	se -8.10	-8.10	0.00	76ENG/MEL
	Literatur	e – Calculated :	= Residual	Reference	trans-Azob	enzene			C ₁₂ H ₁₀ N ₂
Gas phase Δ _t H° =	- 119.30	-114.39	-4.91	76ENG/MEL	(10×C _p .		- (2 × C _B –(N _A)(0 e – Calculated =		
Liquid phas $\Delta_t H^\circ =$	e 172.90	- 164.29	-8.61	76ENG/MEL	Gas phase $\Delta_l H^\circ =$	402.20	402.20	0.00	92DIA/MIN

TABLE 30. Diazenes (14) - Continued

TABLE 31. Azides (6)

trans-Azoben (10×C _B -(I		tinued) (2×C _B -(N _A)($(C_B)_2$ + $(2 \times N)_2$	$C_{12}H_{10}N_2$ A-(C _B))	2-Azidoethan (1×C-(H)		+ (1 × C-(H) ₂ (C	0)(C))+(1×0	C ₂ H ₅ N ₃ O O-(H)(C))
	Literature	e – Calculated	= Residual	Reference		Litera	ture-Calculated	l = Residual	Reference
Liquid phase $\Delta_t H^\circ =$	331.45	331.46	-0.01	77SCH/PET	Liquid phase Δ _t H° =	94.40	94.40	0.00	53FAG/KLE
Solid phase Δ _t H° =	308.60	308.60	0.00	92DIA/MIN	Azidocyclope (4 × C-(H) (1 × azidoc	$_{2}(C)_{2})+(1$	×C-(H)(C) ₂ (N	J ₃))+	C5H9N3
cis-Azobenze (10 × C _B -(1 (1 × cis-azo	$H)(C_B)_2) +$	-(2×C _B -(N _A)($(C_B)_2) + (2 \times N)$	$C_{12}H_{10}N_2$ $A-(C_B))+$			e — Calculated =	- Residual	Reference
(1 ~ 66 - 420		e – Calculated	– Residual	Reference	Gas phase Δ _I H° -	220.90	220.90	0.00	54FAG/MYE
Gas phase Δ _t H° =	450.60	450.60	0.00	92DIA/MIN	Liquid phase $\Delta_l H^\circ =$	179.10	179.10	0.00	54FAG/MYE
Solid phase Δ _t H° =	357.70	357.70	0.00	92DIA/MIN	Azidocyclohe (5 × C-(H) (1 × azidoc	$_{2}(C)_{2})+(1$	× C-(H)(C) ₂ (N : rsc)	(₃))+	C₅H₁1N₃
						Literature	e – Calculated =	- Residual	Reference
					Gas phase $\Delta_i H^\circ =$	154.40	154.40	0.00	54FAG/MYE
					Liquid phase Δ _f H° =	108.40	108.40	0.00	54FAG/MYE
					Azidobenzeno (5 × C _B -(H		tide 1 × C _B -(N ₃))		C ₆ H ₅ N ₃
					*****	Literature	e – Calculated =	Residual	Reference
					Gas phase $\Delta_t H^\circ =$	389.10	389.05	0.05	74PEP/ERL
					Liquid phase $\Delta_t H^\circ =$	344.30	344.30	0.00	29ROT/MUL
					Benzylazide (5×C _B -(H	()(C _B) ₂)+(1×С-(H) ₂ (С _в)	(N ₃))	C ₇ H ₇ N ₃
					_	Literature	e – Calculated =	Residual	Reference
					Gas phase $\Delta_t H^\circ =$	416.10	416.05	0.05	74PEP/ERL

TABLE 31. Azides (6) - Continued

TABLE 32. Cyclic CHN (32)

Benzylazide (5×C _B -(F		$1 \times C - (H)_2(C_B)$	(N ₃))	C ₇ H ₇ N ₃			+ (1 × N-(H)(C))2)+	C ₂ H ₅ N
	Literature	e – Calculated =	= Residual	Reference	(=,		re – Calculated	= Residual	Reference
Liquid phase $\Delta_t H^\circ =$	368.20	368.20	0.00	74PEP/ERL	Gas phase $\Delta_t H^\circ =$	126.48	126.48	0.00	56BUR/GOO
		; Triphenylmet (3×C _B -(C)(C ₁		$C_{19}H_{15}\stackrel{\sim}{N}_3$ (C_{B}) ₃ (N_3))	$C_{\rho}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$	52.51 250.62	52.51 250.62 -183.04 181.05 -73.04	0.00 0.00	69STU/WES 69STU/WES
	Literature	e – Calculated =	= Residual	Reference	mx _f =		- 73.0 4		
Gas phase $\Delta_t H^\circ =$	606.70	606.67	0.03	74PEP/ERL	Liquid phas $\Delta_t H^\circ =$	91.88	91.88	0.00	52NEL/JES
Solid phase $\Delta_t H^\circ =$	486.20	486.15	0.05	74PEP/ERL			$2 \times C - (H)_2(C)(N)$ $\sigma = 2$	∛))+(1×N-(C ₄ H ₉ N H)(C) ₂) +
						Literatui	e – Calculated =	= Residual	Reference
					Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	-3.60 81.13 309.49	-3.60 81.13 309.49 -396.37 115.90 -46.75	0.00 0.00 0.00	59MCC/DOU 59MCC/DOU 59MCC/DOU
					Liquid phas $\Delta_t H^\circ = C_r^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	e -41.20 156.57 204.01	-41.20 156.57 204.01 -502.27 108.55 -43.79	0.00 0.00 0.00	59MCC/DOU 59MCC/DOU 59MCC/DOU
					Pyridine (5×C _B -(1		1×N _I -(C _B)), σ		C₃H₃N
					-	Literatur	e – Calculated =	Residual	Reference
	·				Gas phase $\Delta_f H^\circ = C_r^\circ = S^\circ = \Delta_f S^\circ =$	140.20 78.12 282.80	138.05 78.12 282.80 - 168.08	2.15 0.00 0.00	57MCC/DOU 57MCC/DOU 57MCC/DOU

TABLE 32. Cyclic CHN (32) - Continued

TABLE 32.	Cyclic CHN	(32) -	Continued
TABLE JE.	Cyclic CIII1	(34) -	Continuca

	$(C_B)_2$ + (1	i×N ₁ -(C _B)), σ		C ₅ H ₅ N		$H)(C_B)_2)+($	2×C _B -(C)(C _B ×pyrrole rsc)		C ₆ H ₉ ? H) ₃ (C))+
	Literature	- Calculated -	- Residual	Reference		Literatur	e – Calculated	= Residual	Reference
$C_{\rho}^{\circ} = S^{\circ} =$	100.20 132.72 177.90	95.30 133.15 180.75	4.90 - 0.43 - 2.85	61HUB/FRO 57MCC/DOU 57MCC/DOU	Gas phase $\Delta_t H^\circ =$	39.80	43.45	-3.65	72GOO
$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-270.13 175.84 -70.93			Liquid phas $\Delta_t H^\circ =$	e -16.70	10.11	-6.59	72GOO
1,3,5-Triazine (3 × C _B –(H	$)(N_{\rm I})_2)+(3$	3×N₁–(C _B)) e – Calculated =	= Residual	C ₃ H ₃ N ₃ Reference	(2×N-(C	$(C_B)_2(N) + (C_B)_2(N) + (C_B)_2(N)$	4×C _B -(C)(C _B 2×pyrrole rsc)		
Gas phase Δ _i H° =	225.90	225.90	0.00	82BYS	Solid phase $\Delta_t H^\circ =$	132.30	ulated = Residu	al Referer - 1.48	66COL/SKI
Solid phase Δ _t H° =	171.75	171.75	0.00	82BYS	Piperidine				C _s H ₁₁ N
Pyrrole (4×C _B –(H		(1×N-(H)(C _B); e Calculated =		C₄H₅N ole rsc) Reference	(3×C-(H (1×piper	idine rsc)	× C-(H) ₂ (C)(l e – Calculated		H)(C) ₂) + Reference
Gas phase Δ _t H° =	108.31	108.31	0.00	67SCO/BER	Gas phase $\Delta_t H^\circ =$	-47.20	-47.80	0.60	63BED/BEE
Liquid phase $\Delta_i H^\circ =$		63.11	0.00	67SCO/BER	Liquid phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	e 86.40 179.86 209.97	- 88.38 181.68 209.97 - 632.62 100.24	1.98 -1.82 0.00	72GOO 88MES/TOD 88MES/TOD
N-Methylpyr (4×C _B -(H (1×pyrrol	$(C_B)_2 + ($	(1×N-(C)(C _B):	₂) + (1 × C-(H	C ₅ H ₇ N I) ₃ (N)) +	$\ln K_{\rm f} =$		-40.43		
(1 × pyrror	•	e – Calculated =	= Residual	Reference	Pyridazine $(4 \times C_B - (1 \times C_B))$	H)(C _B) ₂)+($2 \times N_{I}$ –(C_B)) +	(1×N _I -N _I (0	C ₄ H ₄ N ₂ rtho corr))
Gas phase Δ _t H° =	103.14	102.94	0.20	72GOO	Managara and a second	Literatur	e – Calculated :	= Residual	Reference
Liquid phase $\Delta_t H^\circ =$		62.38	0.00	72GOO	Gas phase $\Delta_t H^\circ = C_p^\circ =$	278.30	278.30 74.58	0.00	62TJE2
					Liquid phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	e 224.80	224.80 130.22 188.28 - 287.32 310.47	0.00	62TJE2

TABLE 32.	Cyclic	CHN	(32)		Continued
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Pyrimidine (4×C _B -(H	$I(C_B)_2 + ($	$2 \times N_{\Gamma}(C_B)$		C ₄ H ₄ N ₂	Quinoline (4)		(2×C _{BF} -(C _{BF})	$(C_B)_2) + (1 \times N$	C ₂ H ₇ N N ₁ (C _B))
	Literature	e – Calculated =	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	195.80	193.24 74.58	2.56	77NAB/SAB	Liquid phas $ \Delta_t H^\circ = \\ C_p^\circ = \\ S^\circ = $	141.22 194.89 219.72	143.28 197.55 227.41	- 2.06 - 2.66 - 7.69	88STE/ARC 88STE/ARC 88STE/ARC
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	e 143.80	141.64 130.22 188.28	2.16	77NAB/SAB	$\Delta_t S^\circ = \\ \Delta_t G^\circ = \\ \ln K_t = $		-377.00 255.68 -103.14		
$\Delta_{\rm f}S^{\circ} = \Delta_{\rm f}G^{\circ} = \ln K_{\rm f} =$		-287.32 227.31 -91.69				$I_{2}(C)_{2} + (2$	2×C-(H)2(C)(1 ×pyrrolidine r		C5H11N C)3)+
Pyrazine				C ₄ H ₄ N ₂		Literatui	e – Calculated	= Residual	Reference
•	$H)(C_B)_2) + ($	$(2 \times N_{\Gamma}(C_B))$							
	Literatur	e – Calculated :	= Residual	Reference	Gas phase $\Delta_t H^\circ = C_p^\circ =$		4.41 109.68		
Gas phase $\Delta_t H^\circ = C_p^\circ =$	196.10	193.24 74.58	2.86	62TJE	Liquid phas $\Delta_t H^\circ = C_p^\circ =$	e 161.10	- 28.42 161.09	0.01	76CON/GIN
Liquid phase $\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} =$	e 139.80	141.64 130.22 188.28 -287.32	-1.84	62ТЈЕ	$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = -\infty$		216.60 -625.99 158.22 -63.82	··	
$\Delta_f G^\circ = In K_f =$		227.31 - 91.69			N-Methylpip (3×C-(H (1×N-(C	$()_2(C)_2) + (2)_2$	2×C-(H) ₂ (C)(Niperidine rsc)	√))+(1×C-(I	C ₆ H ₁₃ N H) ₃ (N)) +
	$(2)_2(C)_2 + (2)_2$	2×C-(H)₂(C)(l	N))+(1×N-(1	$C_6H_{13}N$ $H)(C)_2) +$			e – Calculated :	= Residual	Reference
•	nethylenein erature-Cal	nine rsc) culated = Resid	ual Refere	ence	Gas phase $\Delta_t H^\circ =$		-41.11		
Liquid phase $C_p^{\circ} =$	e 205.00	205.03	-0.03	76CON/GIN	Liquid phase $\Delta_t H^\circ = C^\circ = C^\circ$		-75.49 184.00	0.02	Z/CON/GIN
Quinoline (7 × C _B -(1		(2×C _{BF} -(C _{BF})(re – Calculated =		C_9H_7N $N_{I^{-}}(C_B))$ Reference	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1}{2}$	184.93	184.90 222.56 - 756.34 150.01 - 60.51	0.03	76CON/GIN
Gas phase $\Delta_t H^\circ = C_p^\circ =$	200.52	205.87 105.34	-5.35	88STE/ARC					

 $C_6H_{13}N$

C₆H₁₃N

C₆H₇N

TABLE 32. Cyclic CHN (32) - Continued

TABLE 32. Cyclic CHN (32) - Continued

2-Methylpiperidine $(3 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)(N)) + (1 \times C - (H)(C)_2(N)) +$

 $(1 \times -CH_3 \text{ corr (tertiary)}) + (1 \times C - (H)_3(C)) + (1 \times N - (H)(C)_2) +$ (1 × piperidine rsc)

	Literature - Calculated = Residual				
Gas phase Δ _t H° =	-84.40	-80.72	-3.68	72GOO	
Liquid pha	ise			AV.	
$\Delta_t H^\circ =$		-122.02	-2.88	72GOO	
$C_p^{\circ} =$	205.02	216.02	-11.00	76CON/GIN	
S° =		240.89			
$\Delta_f S^\circ =$		-738.01		1	
$\Delta_{\rm f}G^{\circ} =$		98.02			
$lnK_{t} =$		- 39.54			

4-Methylpiperidine

 $(1 \times C - (H)_3(C)) + (1 \times C - (H)(C)_2(N)) +$

 $(1 \times -CH_3 \text{ corr (tertiary)}) + (1 \times C - (H)_2(C)(N)) +$

 $(3 \times C - (H)_2(C)_2) + (1 \times N - (H)(C)_2) + (1 \times piperidine rsc)$

	Literature - Calculated = Residual				
Gas phase $\Delta_t H^\circ =$		-80.72			
Liquid pha	se				
$\Delta_t H^\circ =$		- 122.02			
$C_p^{\circ} =$	209.00	216.02	-7.02	76CON/GIN	
<i>s</i> ° =		240.89			
$\Delta_f S^\circ =$		- 738.01			
$\Delta_f G^{\circ} =$		98.02			
$lnK_f =$		- 39.54			

2-Methylpyridine; 2-Picoline

 $(4 \times C_B - (H)(C_B)_2) + (1 \times C - (H)_3(C)) + (1 \times C_B - (C)(C_B)_2) +$ $(1 \times N_r - (C_B)) + (1 \times N_r - CH_3 (ortho corr)), \sigma = 3$

Literature - Calculated = Residual Reference Gas phase $\Delta_i H^{\circ} =$ 99.20 99.32 -0.1263SCO/HUB $C_p^{\circ} =$ 100.00 99.99 0.01 69STU/WES S° = 325.01 322.83 2.18 69STU/WES $\Delta_f S^\circ =$ -264.36 $\Delta_f G^\circ =$ 178.14 $lnK_f =$ -71.86 Liquid phase $\Delta_i H^{\circ} =$ 56.70 54.69 2.01 63SCO/HUB $C_p^{\circ} = S^{\circ} =$ 158.41 157.05 1.36 63SCO/HUB 217.86 215.68 63SCO/HUB 2.18 $\Delta_f S^\circ =$ -371.51 $\Delta_f G^\circ =$ 165.46 $lnK_f =$ -66.74

3-Methylpyridine; 3-Picoline

C₆H₇N $(4 \times C_B - (H)(C_B)_2) + (1 \times C - (H)_3(C)) + (1 \times C_B - (C)(C_B)_2) +$

 $(1 \times N_{I}-(C_B)), \sigma = 3$

	Literatur	Reference		
Gas phase				
$\Delta_f H^{\circ} =$	106.40	105.62	0.78	63SCO/HUB
$C_p^{\circ} =$	99.58	99.99	-0.41	69STU/WES
<i>S</i> ° =	324.97	322.83	2.14	69STU/WES
$\Delta_f S^\circ =$		-264.36		
$\Delta_f G^\circ =$		184.44		
$lnK_f =$		-74.40		
Liquid pha	ise			
$\Delta_f H^\circ =$	61.90	58.69	3.21	63SCO/GOO
$C_{p}^{\circ} =$	158.70	157.05	1.65	63SCO/GOO
<i>S</i> ° =	216.31	215.68	0.63	63SCO/GOO
$\Delta_f S^\circ =$		-371.51		
$\Delta_f G^{\circ} =$		169.46		
$lnK_f =$		-68.36		

4-Methylpyridine; 4-Picoline

C₆H₇N

 $(4 \times C_B - (H)(C_B)_2) + (1 \times C - (H)_3(C)) + (1 \times C_B - (C)(C_B)_2) +$ $(1 \times N_{\Gamma} - (C_B))$

	Literatur	Reference		
Gas phase $\Delta_t H^\circ =$	104.10	105.62	- 1.52	72GOO
$C_p^{\circ} =$	104.10	99.99	-1.32	72000
T:::J				
Liquid phas $\Delta_t H^\circ =$	se 59.20	58.69	0.51	72GOO
$C_p^{\circ} =$	57.20	157.05	0.51	72000
S° =		215.68		
$\Lambda_{\mathbf{f}} S^{\circ} =$		-371.51		
		169.46		
$\Delta_t G^\circ =$		109.40		

2,3-Dimethylpyridine; 2,3-Lutidine

C₂H₉N

 $(2 \times C - (H)_3(C)) + (2 \times C_B - (C)(C_B)_2) + (3 \times C_B - (H)(C_B)_2) +$ $(1 \times N_{I}-(C_B)) + (1 \times ortho corr, hydrocarbons) +$

 $(1 \times N_1$ -CH₃ (ortho corr))

Literature - Calculated = Residual				Reference	
Gas phase $\Delta_t H^\circ =$	68.30	68.15	0.15	60COX	
Liquid phase $\Delta_t H^\circ =$	19.40	21.34	-1.94	58COX/GUN	

TABLE 32. Cyclic CHN (32) - Continued

TABLE 32. Cyclic CHN (32) - Continued

	$(C_B)_2) + (2_B)_3) + (1 \times m)_4$	$2 \times C - (H)_3(C)$ eta corr, hydr		C ₇ H ₉ N ((C _B) ₂)+	3,4-Dimethylj $(3 \times C_B-(H \times N_F-(C_B))$	$(C_B)_2 + ($	$2 \times C - (H)_3(C)$)+(2×C _B -(C	С ₇Н₉N)(С _В) ₂) +
(IXIII CII	•	Calculated	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_f H^\circ =$	63.90	66.26	-2.36	60COX	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ =$	18.28	25.34 184.45 250.61	- 7.06	58COX/GUN
Liquid phase $\Delta_t H^\circ =$	16.20	18.08	-1.88	58COX/GUN	$\Delta_f S^\circ = \\ \Delta_f G^\circ = \\ \ln K_f = $		-472.89 166.33 -67.10		
• • •	$((C_B)_2) + (1 \times N_B) + (1 \times N_B)$,5-Lutidine 2×C-(H) ₃ (C) ₁ -CH ₃ (ortho	corr))	C_7H_9N $(C_B)_2) +$ Reference	3,5-Dimethylj $(3 \times C_B - (H \times N_I - (C_I \times N_I + C_I \times N_I + (C_I \times N_I + C_I + (C_I \times N_I + C_I + C_I + (C_I \times N_I + C_I + C_I + (C_I \times N_I + C_I + (C_I \times N_I + C_I $	$((C_B)_2) + (B_B) + (1 \times n)$	$2 \times C - (H)_3(C)$		C ₇ H ₉ N)(C _B) ₂) + Reference
					· · · · · · · · · · · · · · · · · · ·				Reference
Gas phase Δ _i H° =	66.50	66.89	-0.39	60COX	Gas phase $\Delta_i H^\circ = C_p^\circ =$	72.80	72.56 122.57	0.24	60COX
Liquid phase $\Delta_t H^\circ =$	18.70	18.08	0.62	58COX/GUN	Liquid phase $\Delta_t H^\circ = C_p^\circ =$	22.50	22.08 180.95	0.42	58COX/GUN
	$((C_B)_2) + (B_B) + (1 \times m)$	2×C-(H)3(C) teta corr, hydr		C_7H_9N $C_7(C_B)_2$	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = -\infty$		250.61 -472.89 163.07 -65.78		
	Literature	e – Calculated	= Residual	Reference	Octahydroazo	wine			C7H15N
Gas phase Δ _t H° =	58.70	59.96	-1.26	60COX		$_{2}(C)_{2})+(2$	× C-(H) ₂ (C)(N : rsc)	N))+(1×N-(I	$H)(C)_2) +$
						Literat	ure-Calculated	d = Residual	Reference
Liquid phase $\Delta_t H^\circ =$	12.72	14.08	-1.36	58COX/GUN	Liquid phase $C_p^{\circ} =$	230.00	230.00	0.00	76CON/GIN
3,4-Dimethyl (3×C _B -(H (1×N _I -(C	$(C_B)_2 + (C_B)_1 + (1 \times a)_2$	2×C-(H)₃(C) rtho corr)				$_{2}(C)_{2})+(1$	×C-(H) ₃ (C))+ peridine rsc)	+ (3×C−(H) ₂ (C ₈ H ₁₇ N C)(N)) +
	Literature	e – Calculated	= Residual	Reference		Literature	- Calculated =	= Residual	Reference
Gas phase $\Delta_l H^\circ = C_p^\circ =$	70.08	74.45 128.26	-4.37	60COX	Gas phase $\Delta_t H^\circ =$		- 90.04		

TABLE 32. Cyclic CHN (32) - Continued

TABLE 33. Amides (28)

TABLE 32. Cyclic CFIN (32) — Continued	TABLE 33. Annues (20)
N-Propylpiperidine (Continued) $C_8H_{17}N$ $(4 \times C-(H)_2(C)_2) + (1 \times C-(H)_3(C)) + (3 \times C-(H)_2(C)(N)) + (1 \times N-(C)_3) + (1 \times piperidine rsc)$	Methanamide; Formamide CH ₃ NC (1×CO-(H)(N))+(1×N-(H) ₂ (CO))
Literature – Calculated = Residual Reference	Literature - Calculated = Residual Reference
Liquid phase $\Delta_t H^\circ = -147.00 - 132.02 - 14.98$ 70PRO/KRE $C_p^\circ = 245.74$	Gas phase $\Delta_t H^\circ = -186.19 - 187.39$ 1.20 58BAU/GUN $C_p^\circ = 46.00$
$S^{\circ} = 287.32$ $\Delta_t S^{\circ} = -964.20$ $\Delta_t G^{\circ} = 155.46$ $\ln K_t = -62.71$	Liquid phase $\Delta_t H^\circ = -251.00 -251.90 0.90 58BAU/GUN$ $C_p^\circ = 108.11 108.11 0.00 77VOR/PRI$
Pyrrolizidine; 1-Azabicyclo[3.3.0]octane $C_7H_{13}N$ $(4 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(C)(N)) + (1 \times C - (H)(C)_2(N)) +$ $(1 \times Pyrrolizidine rsc) + (1 \times N - (C)_3)$	Ethanamide; Acetamide C_2H_3NC $(1 \times C - (H)_3(C)) + (1 \times CO - (C)(N)) +$ $(1 \times N - (H)_2(CO))$ (amides, ureas)), $\sigma = 3$
Literature - Calculated = Residual Reference	Literature – Calculated = Residual Reference
Gas phase $\Delta_t H^{\circ} = -3.90 -3.90 0.00 81 \text{KOZ/TIM}$	Gas phase $\Delta_t H^\circ = -238.30 -238.52$ 0.22 75BAR/PIL
Liquid phase $\Delta_t H^{\circ} = -48.30 - 48.30 0.00 81KOZ/TIM$	$C_r^o = 63.22$ 65.23 -2.01 67PUR/SIR $S^o = 272.21$ 263.14 9.07 67PUR/SIR $\Delta_t S^o = -273.04$ $\Delta_t G^o = -157.11$ $\ln K_t = 63.38$
(cis -3,7a-H)-(cis -5,7a-H)-3,5-Dimethylpyrrolizidine $(4 \times C-(H)_2(C)_2) + (3 \times C-(H)(C)_2(N)) + (1 \times N-(C)_3) + (2 \times C-(H)_3(C)) + (2 \times -CH_3 \text{ corr (tertiary)}) + (1 \times 3,5-Dimethylpyrrolizidine rsc)$	Liquid phase $\Delta_t H^\circ = -296.51$ $C_\rho^\circ = 128.65$
Literature – Calculated – Residual Reference	Solid phase
Gas phase $\Delta_t H^{\circ} = -66.70 - 66.70 = 0.00$ 81KOZ/TIM	$\Delta_t H^\circ = -317.00 -306.59 -10.41$ 75BAR/PIL $C_p^\circ = 91.30$ 90.95 0.35 84NUR/BER $S^\circ = 115.00$ 114.69 0.31 84NUR/BER $\Delta_t S^\circ421.49$ $\Delta_t G^\circ = -180.92$ $\ln K_f = 72.98$
Liquid phase $\Delta_t H^\circ = -114.40 - 114.40 0.00 81KOZ/TIM$	
	Propanamide; Propionamide $C_3H_7NO_1$ (1×C-(H) ₂ (C)) + (1×C-(H) ₂ (CO)(C)) + (1×CO-(C)(N)) + (1×N-(II) ₂ (CO))
	Literature - Calculated = Residual Reference
	Gas phase $\Delta_t H^\circ = -258.99 -260.36$ 1.37 75BAR/PIL $C_p^\circ = 89.92$
	Liquid phase $\Delta_t H^{\circ} = -320.65$ $C_p^{\circ} = 157.94$

TABLE 33. Amides (28) - Continued

Propanamide; Propionamide (Continued) C_3H_7NO $(1 \times C-(H)_3(C)) + (1 \times C-(H)_2(CO)(C)) + (1 \times CO-(C)(N)) + (1 \times N-(H)_2(CO))$	Butanamide; Butyramide $(1 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) +$	
Literature - Calculated = Residual Reference	Literature – Calculated = Residual	Reference
Solid phase $\Delta_t H^\circ = -338.20 -334.49 -3.71$ 75BAR/PIL $C_p^\circ = 112.87$ $S^\circ = 139.42$ $\Delta_t S^\circ = -533.07$	Gas phase $\Delta_0 H^{\circ} = -279.20 -280.99$ 1.79 $C_p^{\circ} = 112.81$	75BAR/PIL
$\Delta_f G^{\circ} = -175.56$ $\ln K_f = 70.82$	Liquid phase $\Delta_t H^{\circ} = -346.38$ $C_p^{\circ} = 188.36$	
2-Methylpropanamide C ₄ H ₉ NO	Galida Laca	
$(2 \times C-(H)_3(C)) + (2 \times -CH_3 \text{ corr (tertiary)}) + (1 \times C-(H)(CO)(C)_2) + (1 \times CO-(C)(N)) + (1 \times N-(H)_2(CO))$	Solid phase $\Delta_t H^\circ = -365.53 -363.90 -1.63$ $C_p^\circ = 134.79$	75BAR/PIL
Literature - Calculated = Residual Reference	$S^{\circ} = 162.43$ $\Delta_i S^{\circ} = -646.37$ $\Delta_i G^{\circ} = -171.18$	
Gas phase $\Delta_t H^\circ = -282.60 -285.55$ 2.95 89ABB/JIM	$\ln K_t = 69.05$	
Liquid phase $\Delta_t H^\circ = -352.37$ $C_p^\circ = 182.54$	Pentanamide $ (1 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)_2) + (1 \times C - $	C ₅ H ₁₁ NO CO)(C)) +
Solid phase	Literature – Calculated = Residual	Reference
$\Delta_t H^\circ = -368.60 - 367.84 - 0.76$ 89ABB/JIM $C_\rho^\circ = 77.89$	Gas phase $\Delta_t H^\circ = -290.20 -301.62$ 11.42 $C_p^\circ = 135.70$	59DAV/JON
2,2-Dimethylpropanamide $(3 \times C-(H)_1(C)) + (3 \times -CH_1 \text{ corr (quaternary)}) + (1 \times C-(CO)(C)_3) + (1 \times CO-(C)(N)) + (1 \times N-(H)_2(CO))$	Liquid phase $\Delta_t H^\circ = -372.11$	
Literature - Calculated = Residual Reference	$C_{\rho}^{\circ} = 218.78$	
Gas phase $\Delta_t H^\circ = -313.10 -312.79 -0.31$ 88ABB/JIM	Solid phase $\Delta_t H^\circ = -379.49 -393.31$ 13.82 $C_p^\circ = 156.71$ $S^\circ = 185.44$	56YOU/KEI
Liquid phase $\Delta_t H^\circ = -378.75$ $C_r^\circ = 209.60$	$\Delta_{f}S^{\circ} = -759.67$ $\Delta_{f}G^{\circ} = -166.81$ $\ln K_{f} = 67.29$	
Solid phase $\Delta_t H^\circ = -399.70 -389.10 -10.60$ 89ABB/JIM $C_p^\circ = 111.75$	Hexanamide $(1 \times C - (H)_3(C)) + (3 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2)$	C ₆ H ₁₃ NO CO)(C))+
	Literature – Calculated = Residual	Reference
	Gas phase $\Delta_t H^{\circ} = -324.20 -322.25 -1.95$ $C_p^{\circ} - 158.59$	73LEB/KAT2

TABLE 33	. Amides	(28) —	Continued
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Hexanamide (Continued) $(1 \times C - (H)_3(C)) + (3 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2)$ $(1 \times CO - (C)(N)) + (1 \times N - (H)_2(CO))$	CO)(C))+	(2×C-(H	•	mide; N,N-Dim ×CO-(H)(N)) ternary))	•	
Literature – Calculated = Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid phase $\Delta_b H^{\circ} = -397.90 -397.84 -0.06$ $C_p^{\circ} = 249.20$	73LEB/KAT2	Gas phase $\Delta_t H^\circ =$	191.70 	-173.03	- 18.67	61GEL
Solid whose	IS F	Liquid phas $\Delta_t H^\circ =$	e 239.20	- 230.00	- 9.20	72VAS/ZHI
Solid phase $\Delta_t H^\circ = -423.42 -422.72 -0.70$ $C_p^\circ = 178.63$ $S^\circ = 208.45$	73LEB/KAT2	$C_{\rho}^{\circ} =$	152.00	151.99	0.01	74VIS/SOM
$\Delta_{t}S^{\circ} = -872.97$ $\Delta_{t}G^{\circ} = -162.44$ $\ln K_{f} = 65.53$			I)3(C))+(1	-Ethylacetamid ×C-(H) ₂ (C)(N		C4H4NO ()(C)(CO)) +
Octanamide	C ₈ H ₁₇ NO		Literatu	re – Calculated	= Residual	Reference
$(1 \times C - (H)_3(C)) + (5 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2) +$		Gas phase Δ _t H° =		-262.36		
Literature - Calculated = Residual	Reference			202.50		
Gas phase		Liquid phas $\Delta_f H^\circ =$	e	-328.12		
$\Delta_l H^{\circ} = -362.80 - 363.51 0.71$ $C_p^{\circ} = 204.37$	59DAV/JON	$C_p^{\circ} =$	179.91	176.05	3.86	71KON/WAD
Liquid phase $\Delta_t H^{\circ} = -449.30$ $C_{\rho}^{\circ} = 310.04$		(2×C-(H	1)3(C))+(1	N-Propylacetam × C-(H) ₂ (C) ₂) 1 × C-(H) ₂ (C)(1	+ (1 × N-(H)(0	C5H11NO C)(CO)) +
Solid phase			Literatu	re – Calculated	= Residual	Reference
$\Delta_{i}H^{\circ} = -473.10 -481.54 8.44$ $C_{p}^{\circ} = 222.47$ $S^{\circ} = 254.47$ $\Delta_{i}S^{\circ} = -1099.57$	56YOU/KEI	Gas phase $\Delta_t H^\circ =$		- 282.99		
$\Delta_t G^{\circ} = -153.70$ $\ln K_t = 62.00$		Liquid phas $\Delta_t H^\circ = C_p^\circ =$	e 207.11	-353.85 206.47	0.64	71KON/WAD
N-Methylmethanamide; N-Methylformamide	C₂H₅NO	•				
$(1 \times C - (H)_3(C)) + (1 \times N - (H)(C)(CO)) + (1 \times CO - (H)_3(C)) $	(H)(N)) Reference			; N-Isopropylac ×C-(H)(C) ₂ (N		C ₅ H ₁₁ NO
		(2×-CH₃ (1×CO-(iary)) + (1 × N-((H)(C)(CO))+	
Gas phase $\Delta_t H^\circ = -182.93$			Literatu	re – Calculated	= Residual	Reference
Liquid phase $\Delta_{r}H^{\circ} = -252.71$ $C_{p}^{\circ} = 125.10$ 125.09 0.01	79VIS/SOM	Gas phase $\Delta_t H^\circ =$		- 297.54		
		Liquid phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} =$	e 210.90	-363.94 210.39	0.51	71KON/WAD

TABLE 33. Amides (28) - Continued

	1)(C)(CO))	+(1×CO-(C)	(N))		(17.11 (0)2(00)) 1 (2 X -CH3 COH	(quaternary))	
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase Δ _i H° =	- 304.80	-303.62	-1.18	65WAD	Gas phase $\Delta_i H^\circ =$		- 246.00		-
Liquid phase $\Delta_t H^\circ = C_\rho^\circ =$	se - 380.90 236.00	-379.58 236.89	-1.32 -0.89	62WAD 71KON/WAD	Liquid phase $\Delta_t H^\circ = C_p^\circ =$	209.20	- 298.75 201.82	7.38	71KON/WAD
Butylace	tamide	ethanamide; N- ×C-(C)3(N)) +		C ₆ H ₁₃ NO rr (quaternary))+) ₃ (C))+(2	× C-(H)2(C)2) 1 × N-(H)(C)(C		C ₆ H ₁₃ N((CO)(C))+
(1×N-(1	H)(C)(CO))	+(1×CO-(C)	(N))			Literatui	e – Calculated:	= Residual	Reference
	Literatur	re – Calculated	= Residual	Reference	Gas phase $\Delta_t H^\circ =$		-297.16		
Gas phase $\Delta_t H^\circ =$		-331.97			Liquid phase	e			
Liquid pha $\Delta_t H^\circ = C_p^\circ =$	se	-400.61 238.25			$\Delta_{\mathfrak{l}}H^{\circ} = C_{\mathfrak{p}}^{\circ} =$	228.90	-372.92 235.76	- 6.86	71KON/WAD
Solid phase $\Delta_t H^\circ = C_p^\circ =$	189.95	-403.41 188.66	1.29	71KON/WAD) ₃ (C))+(4)(C)(CO))	$ \times C - (H)_2(C)_2 $ $ + (1 \times CO - (C))_2 $ $ + (1 \times C)_2 $	(N))+(1×C-	
(2×C-(; N-Methylpro ₁ ×C-(H) ₂ (CO)		C ₄ H ₉ NO (C)(N))+	Gas phase $\Delta_t H^\circ =$		- 366.72		
(20,11)	11)(0)(00)		= Residual	Reference	Liquid phase $\Delta_t H^\circ =$	e	-455.18		
	Literatu	re - Calculated	- Kesiduai		$C_p^{\circ} =$		327.02		
Gas phase Δ _t H° =	Literatu	- 255.90	- Nesidual		$C_p^{\circ} =$ Solid phase $\Delta_t H^{\circ} =$	- 465.10	-477.42	12.32	66SKU/BON
Gas phase $\Delta_t H^\circ =$ Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$			4.16	71KON/WAD	$C_p^{\circ} =$ Solid phase $\Delta_t H^{\circ} =$ $C_p^{\circ} =$		-477.42 269.42		
$\Delta_t H^{\circ} =$ Liquid pha $\Delta_t H^{\circ} =$	se	- 255.90 - 321.46			$C_{\rho}^{\circ} =$ Solid phase $\Delta_t H^{\circ} =$ $C_{\rho}^{\circ} =$ N-Butyldiace $(3 \times C - (H^{\circ}))$	etamide; N) ₃ (C)) + (2	-477.42	mine + (1 × C-(H) ₂ (C _s H ₁₅ NO ₂
$\Delta_t H^{\circ} =$ Liquid pha $\Delta_t H^{\circ} =$	se	- 255.90 - 321.46			$C_{\rho}^{\circ} =$ Solid phase $\Delta_t H^{\circ} =$ $C_{\rho}^{\circ} =$ N-Butyldiace $(3 \times C - (H^{\circ}))$	etamide; N) ₃ (C)) + (2 C)(N)) + (1	- 477.42 269.42 -Butyldiacetyla × C-(H) ₂ (C) ₂)-	mine + (1 × C–(H) ₂ ()	C ₈ H ₁₅ NO ₂
$\Delta_t H^{\circ} =$ Liquid pha $\Delta_t H^{\circ} =$	se	- 255.90 - 321.46			Solid phase $\Delta_t H^\circ = C_\rho^\circ =$ N-Butyldiace $(3 \times C - (H)$ $(2 \times CO - (G))$ Gas phase	etamide; N) ₃ (C)) + (2 C)(N)) + (1	-477.42 269.42 -Butyldiacetylai × C-(H) ₂ (C) ₂)- l × N-(C)(CO) ₂	mine + (1 × C–(H) ₂ ()	C ₈ H ₁₅ NO ₂ C)(N)) +

TABLE 33. Amides (28) - Continued

Acetanilide; N-Phenylethanamide; N-Phenylacetamide	C ₈ H ₉ NO
$(1 \times C - (H)_3(C)) + (1 \times CO - (C)(N)) + (1 \times N - (H)(C_B)(CO))$	+
$(1 \times C_{n-1}(N)(C_{n})_{n}) + (5 \times C_{n-1}(H)(C_{n})_{n})$	

128.90 –	128.61 –	0.29	55AIH
			62WAD 86NIL/WAD
	209.60 –	209.60 – 202.44 –	209.60 -202.44 -7.46

Butanediamide; Succinamide $C_4H_8N_2O_2\\ (2\times N-(H)_2(CO))+(2\times CO-(C)(N))+(2\times C-(H)_2(CO)(C))$

	Literature – Calculated	= Residual 	Reference
Gas phase			
$\Delta_{\ell}H^{\circ} =$	-436.20		
C _P =	128.38		
Liquid phase	e		
$\Delta_i H^\circ =$	- 546.08		
C _p =	242.92		
Solid phase			
$\Delta_t H^{\circ} = -$	-581.20 -575.50	-5.70	57TAM/LAM
$C_n^{\circ} =$	90.84		
S° =	165.46		
$\Delta_f S^\circ =$	-776.33		
$\Delta_{\rm f}G^{\circ} =$	-344.04		
$lnK_f =$	138.78		

Propanediamide; Malonamide $C_3H_6N_2O_2$ $(2 \times N-(H)_2(CO)) + (2 \times CO-(C)(N)) + (1 \times C-(H)_2(CO)_2)$

Literatu	re – Calculated =	- Residual	Reference
Gas phase Δ _i H° =	-423.24		
Liquid phase			
$\Delta_{\rm f}H^{\circ} =$	- 520.85		
C _p =	199.90		
Solid phase			
$\Delta_{\rm f}H^{\circ} = -546.10$	-538.80	-7.30	55TAV/LAM

N,N-Dimethylethanamide; N,N-Dimethylacetamide $(2 \times C - (H)_3(N)) + (1 \times C - (H)_3(CO)) + (1 \times CO - (C)(N)) + (1 \times N - (C)_2(CO)) + (2 \times - CH_3 \text{ corr (quaternary)})$

Literatu	re – Calculated	= Residual	Reference
Oas phase $\Delta_t H^\circ = -232.60$	- 224.16	- 8.44	74GUT
Liquid phase $\Delta_t H^\circ = -278.30$ $C_p^\circ =$	-274.61 172.53	-3.69	72VAS/ZHI

$\begin{array}{ll} N\text{-}Acetyl-N\text{-}butylacetamide} & C_8H_{15}NO_2\\ (2\times C-(H)_3(CO)) + (2\times CO-(C)(N)) + (1\times N-(C)(CO)_2) + \\ (1\times C-(H)_2(C)(N)) + (2\times C-(H)_2(C)_2) + (1\times C-(H)_3(C)) \end{array}$

Gas phase $\Delta_t H^\circ = -474.50 \qquad -474.50 \qquad 0.00 \qquad 65 \text{WAD}$ Liquid phase	 Literature – Calculated = Residual			Reference	
		-474.50	0.00	65WAD	
$\Delta_t H^\circ = -538.90 -538.89 -0.01$ 65WAD		- <i>5</i> 38.89	-0.01	65WAD	

$\begin{tabular}{lll} \textbf{Benzamide} & & & & & & & & \\ & (5 \times C_B-(H)(C_B)_2) + (1 \times C_B-(CO)) + (1 \times CO-(C_B)(N)) + \\ & & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ &$

L	Literature-Calculated = Residual		Referei	nce
Solid phas	se			
$\Delta_{\rm f} H^{\circ} =$	-202.14	- 202.20	0.06	90STE/CHI
$C_p^{\circ} =$	153.82	153.86	-0.04	90STE/CHI

1-Adamantyl carboxamide; Tricyclo[3.3.1.1^{3,7}]decane-

 $\begin{array}{l} \textbf{1-carboxamide} & \textbf{C}_{11}\textbf{H}_{17}\textbf{NO} \\ (4 \times \textbf{C}-(\textbf{H})(\textbf{C})_3) + (5 \times \textbf{C}-(\textbf{H})_2(\textbf{C})_2) + (1 \times \textbf{C}-(\textbf{H})(\textbf{CO})(\textbf{C})_2) + \\ (1 \times \textbf{CO}-(\textbf{C})(\textbf{N})) + (1 \times \textbf{N}-(\textbf{H})_2(\textbf{CO})) + (1 \times \textbf{Adamantane rsc}) \end{array}$

Literatu	Literature – Calculated = Residual				
Gas phase $\Delta_t H^\circ = -319.00$	-310.48	-8.52	89ABB/JIM		
Solid phase $\Delta_t H^\circ = -427.20$	-437.47	10.27	89ABB/JIM		

ESTIMATION OF THERMODYNAMIC PROPERTIES OF ORGANIC COMPOUNDS

TABLE 34. Ureas (24)

TABLE 34. Ureas (24) - Continued

Urea (2×N-(I	H)2(CO) (an	nides, ureas))⊣	· (1×CO-(N)	CH_4N_2O 2), $\sigma = 2$	Trimethylurea $(3 \times C-(H)_3(N)) + (1$ $(1 \times CO-(N)_2) + (1 \times CO-(N)_2)$			
	Literatur	e – Calculated	= Residual	Reference		re – Calculated =		Reference
Gas phase								
$\Delta_{\epsilon}H^{\circ} = C_{p}^{\circ} = S^{\circ} =$	-235.51 66.40 266.98	-237.00 66.40 266.74	1.49 0.00 0.24	90KAB/MIR 83FRE/GUS 83FRE/GUS	Gas phase $\Delta_t H^\circ =$	-218.18		
$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		- 294.17 - 149.29 60.22			Liquid phase $\Delta_l H^\circ =$	- 297.21		
Liquid pha $\Delta_t H^\circ =$	se -320.20	-318.30	1.90	72ZOR/HUR	Solid phase $\Delta_t H^\circ = -330.50$	-306.82 -2	23.68 56TA\	//LAM
Solid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	e -333.59 93.08 104.93	- 333.60 93.00 105.00 - 455.90 - 197.67	0.01 0.08 - 0.07	90KAB/MIR 86KOZ/DAL 86KOZ/DAL	Tetramethylurea (4×C-(H) ₃ (N))+(2 (4×-CH ₃ corr (qual	2×N−(C)2(CO)) ternary)) re − Calculated =		$C_5H_{12}N_2O$ $N)_2) +$ Reference
	H)2(CO) (as	79.74 mides, ureas))-			Gas phase $\Delta_t H^\circ = -205.57$	- 208.28	2.71	90KAB/MIR
(1×N-(,,,,,	(amides, ureas re – Calculated		() ₃ (N)) Reference	Liquid phase $\Delta_1 H^\circ = -262.17$	- 274.50	12.33	87SIM/KAB
Gas phase Δ _i H° =	-233.48	- 232.54	- 0.94	90KAB/MIR	Solid phase $\Delta_t H^\circ = -276.27$	- 297.46	21.19	72ZOR/HUR
Liquid pha Δ _t H° =		-319.11	0.30	72ZOR/HUR	Ethylurea $(1 \times C - (H)_3(C)) + (1$	×C-(H) ₂ (C)(N))+	C ₃ H ₈ N ₂ O
Solid phas $\Delta_t H^\circ = C_p^\circ =$	e - 332.78	-324.89 139.95	- 7.89	87SIM/KAB	$(1 \times N-(H)(C)(CO)$ $(1 \times N-(H)_2(CO))$ (and Literatus)		, , ,	N) ₂) + Reference
N,N-Dimet (2×C-((1×N-($(H)_3(N)) + (1)_2(CO)$ (a)	×N-(C)₂(CO)		C ₃ H ₈ N ₂ O N) ₂) +	Gas phase $\Delta_t H^\circ = -257.46$	- 260.84	3.38	90KAB/MIR
(2x-CF	H₃ corr (qua Literatu	ternary)) re – Calculated	= Residual	Reference	Liquid phase $\Delta_t H^\circ =$	- 349.91		
Gas phase Δ _t H° =	-219.96	- 222.64	2.68	90KAB/MIR	Solid phase $\Delta_t H^{\circ} = -357.76$ $C_p^{\circ} =$	-358.89 161.87	1.13	87SIM/KAB
Liquid pha $\Delta_t H^\circ =$	ase 296.09	- 296.40	0.31	72ZOR/HUR				
Solid phas $\Delta_t H^\circ =$	e -319.06	-315.53	-3.53	87SIM/KAB				

TARIF	34	Hreas	(24)	 Continued
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TABLE 34. Ureas (24) — Continue	ed	TABLE 34. Ureas (24) — Continued					
N,N-Diethylurea $(2 \times C-(H)_3(C)) + (2 \times C-(H)_2(C)(N)) + (1 \times N-(C)(1 \times CO-(N)_2) + (1 \times N-(H)_2(CO))$ (amides, ureas))	N-n-Butylurea (1×C-(H) ₃ (C))+(2× (1×N-(H)(C)(CO) ((1×N-(H) ₂ (CO) (am	amides, ureas))+(1>				
Literature – Calculated = Residual	Reference	Literature	e – Calculated = Resid	lual Reference			
Gas phase $\Delta_t H^{\circ} = -272.31 -270.12 -2.19$	90KAB/MIR	Gas phase $\Delta_t H^\circ = -313.58$	-302.10 -11	.48 90KAB/MIR			
Liquid phase $\Delta_t H^\circ = -349.22$		Liquid phase Δ _t H° =	-401.37				
Solid phase $\Delta_t H^\circ = -372.21 -374.83$ 2.62	87SIM/KAB	Solid phase $\Delta_t H^\circ = -419.48$ $C_p^\circ =$	-417.71 -1 205.71	.77 87SIM/KAB			
Tetraethylurea $(4 \times C - (H)_3(C)) + (4 \times C - (H)_2(C)(N)) + (2 \times N - (C)(1 \times CO - (N)_2))$ $Literature - Calculated = Residual$	C ₃ H ₂₆ N ₂ O (2) ₂ (CO)) + Reference	N-sec-Butylurea $(2 \times C - (H)_3(C)) + (1 \times C - (H)(C)(C)$ $(1 \times C - (H)_3) = (1 \times C - (H)(C)(C)$ $(1 \times C - (H)_2) = (1 \times C - (H)(C)(C)$	amides, ureas)) + ary)) + $(1 \times CO - (N)_2)$				
Gas phase $\Delta_i H^\circ = -316.43 -303.24 -13.19$	90KOZ/SIM		e – Calculated = Resid	lual Reference			
Liquid phase $\Delta_l H^\circ = -380.04 -380.14 0.10$	90KOZ/SIM	Gas phase $\Delta_t H^\circ = -307.03$	-314.39 7	.36 90KAB/MIR			
Solid phase $\Delta_t H^\circ = -403.04 -416.06$ 13.02	90KOZ/SIM	Liquid phase $\Delta_t H^\circ =$	- 409.28				
N-Isopropylurea $(2 \times C - (H)_3(C)) + (1 \times C - (H)(C)_2(N)) + (2 \times - CH_3 \text{ corr (tertiary)}) +$	C ₄ H ₁₀ N ₂ O	Solid phase $\Delta_t H^{\circ} = -413.06$	-417.28 4	.22 87SIM/KAB			
(1×N-(H)(C)(CO) (amides, ureas))+(1×CO-(1 (1×N-(H) ₂ (CO) (amides, ureas)) Literature - Calculated = Residual	N) ₂) + Reference	N-tert - Butylurea (3 × C-(H) ₃ (C)) + (1 × (1 × N-(H)(C)(CO) ((1 × N-(H) ₂ (CO) (am	amides, ureas))+(1>	$C_3H_{12}N_2O$ CH ₃ corr (quaternary)) + $(CO-(N)_2)$ +			
Gas phase $\Delta_0 H^\circ = -289.79 -296.02$ 6.23	90KAB/MIR	Literature	e – Calculated = Resid	lual Reference			
Liquid phase $\Delta_0 H^\circ = -385.73$		Gas phase $\Delta_t H^\circ = -314.03$	-330.45 16	.42 90KAB/MIR			
Solid phase $\Delta_t H^\circ = -389.49 -390.21$ 0.72	87SIM/KAB	Liquid phase $\Delta_t H^\circ =$	-422.40				
		Solid phase $\Delta_t H^\circ = -414.73$ $C_\rho^\circ -$	-430.42 15.	.69 87SIM/KAB			

TABLE 34. Ureas (24) - Continued

TABLE 34. Ureas (24) - Continued

	Literatur	e – Calculated =	= Residual	Reference	
	Literatur	Calculated			Literature-Calculated = Residual Reference
Gas phase $\Delta_t H^\circ =$	- 404.21	-400.38	-3.83	90KAB/MIR	Solid phase $\Delta_t H^\circ = -106.80 - 113.99$ 7.19 52MED/T
Liquid pha $\Delta_t H^\circ =$	se	-504.00			N,N'-Dimethyl-N,N'-diphenylurea C ₁₅ H ₁
Solid phase $\Delta_t H^\circ = C_p^\circ =$	e 499.81	- 514.58 288.42	14.77	87SIM/KAB	$(2 \times C - (H)_3(N)) + (10 \times C_B - (H)(C_B)_2) + (2 \times C_B - (N)) + (1 \times CO - (N)) + (2 \times N - (C)(C_B)(CO))$
					Literature-Calculated = Residual Reference
	$(H)(C_B)_2) + \epsilon$	(1 × C _B -(N)(C _B) N-(H) ₂ (CO) (a			Solid phase $\Delta_t H^\circ = -73.20 - 67.78 - 5.42$ 52MED/T
	Literatur	e – Calculated =	= Residual	Reference	
Gas phase Δ _t H° =		- 127.09			$\label{eq:continuous} N'\text{-Ethyl-N,N-diphenylurea} \\ (10 \times C_B-(H)(C_B)_2) + (2 \times C_B-(N)(C_B)_2) + (1 \times N-(C_B)_2(CO)) + \\ (1 \times CO-(N)_2) + (1 \times N-(H)(C)(CO) \text{ (amides, ureas))} + \\ (1 \times C-(H)_2(C)(N)) + (1 \times C-(H)_3(C)) \\$
Solid phase $\Delta_t H^\circ = C_p^\circ =$	e -231.50	-229.45 181.15	-2.05	87KUL/KIP	Literature-Calculated = Residual Reference
					Solid phase $\Delta_t H^{\circ} = -152.60 - 147.99 - 4.61$ 52MED/T
N,N'-Diphe (10×C _{B'} (1×CO-	-(H)(C _B) ₂) + -(N) ₂)	- (2 × C _B –(N)(C re – Calculated =		$C_{13}H_{12}N_2O$ (H)(C _B)(CO))+ Reference	N,N'-Diethyl-N,N'-diphenylurea $C_{17}H_2$ $(10 \times C_B-(H)(C_B)_2) + (2 \times C_B-(N)) + (2 \times C-(H)_3(C)) + (2 \times C-(H)_2(C)(N)) + (1 \times CO-(N)_2) + (2 \times N-(C)(C_B)(CO))$
(10×C _B (1×CO-	-(H)(C _B) ₂) + -(N) ₂)			$(H)(C_B)(CO))+$	
$(10 \times C_B)$	-(H)(C _B) ₂) + -(N) ₂)			$(H)(C_B)(CO))+$	$(10 \times C_{B}-(H)(C_{B})_{2}) + (2 \times C_{B}-(N)) + (2 \times C-(H)_{3}(C)) + (2 \times C-(H)_{2}(C)(N)) + (1 \times CO-(N)_{2}) + (2 \times N-(C)(C_{B})(CO))$
(10×C _B) (1×CO-	–(H)(C _B) ₂) + -(N) ₂) Literatur	e – Calculated =		$(H)(C_B)(CO))+$	$(10 \times C_B - (H)(C_B)_2) + (2 \times C_B - (N)) + (2 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)(N)) + (1 \times CO - (N)_2) + (2 \times N - (C)(C_B)(CO))$ $Literature-Calculated = Residual \qquad Reference$ $Solid phase$ $\Delta_t H^\circ = -132.30 -135.78 \qquad 3.48 \qquad 43PRO/GI$
$(10 \times C_B)$ $(1 \times CO$ Gas phase $\Delta_t H^\circ =$ Solid phase $\Delta_t H^\circ =$ $C_p^\circ =$ N,N-Diphe $(10 \times C_B)$	e -(H)(C _B) ₂) + -(N) ₂) Literatur e -116.83	- 17.18 - 125.30	= Residual 8.47 8.9 ₂) + (1 × N-((H)(C _B)(CO)) + Reference 87SIM/KAB C ₁₃ H ₁₂ N ₂ O (C _B) ₂ (CO)) +	$(10 \times C_B - (H)(C_B)_2) + (2 \times C_B - (N)) + (2 \times C - (H)_3(C)) +$ $(2 \times C - (H)_2(C)(N)) + (1 \times CO - (N)_2) + (2 \times N - (C)(C_B)(CO))$ $Literature-Calculated = Residual \qquad Reference$ Solid phase

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Table 34. Ureas (24) — Continued	TABLE 3	34. L	Jreas	(24)	- (Continued
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TABLE 35. Amino acids (38)

$ \begin{array}{c} \textbf{Tetraphenylurea} & \textbf{C}_{25}\textbf{H}_{20}\textbf{N}_{2}\textbf{O} \\ (20 \times \textbf{C}_{B} - (\textbf{H})(\textbf{C}_{B})_{2}) + (4 \times \textbf{C}_{B} - (\textbf{N})) + (2 \times \textbf{N} - (\textbf{C}_{B})_{2}(\textbf{CO})) + \\ (1 \times \textbf{CO} - (\textbf{N})_{2}) \end{array} $				C ₂₅ H ₂₀ N ₂ O (CO))+	$(1 \times N - (H$	Aminoethanoic acid; Glycine $(1 \times N-(H)_2(C)) + (1 \times C-(H)_2(CO)(N)) + (1 \times C-(H)_2(CO)(N)) + (1 \times C-(H)(CO)) + (1 \times C-(H)(CO)) + (1 \times C-(H)(CO)(N)) + (1 \times$				
Lite	erature-Calc	ulated = Resid	ual Refere	nce	***	Literatu	re – Calculated	= Residual	Reference	
Solid phase Δ _t H° =	168.00	88.20	79.80	1897HAU	Gas phase $\Delta_t H^\circ =$	375.30 	- 375.39	0.09	77NGA/SAB	
	$(N)_2)+(1\times 1)$	1 × CO-(C)(N) N-(H) ₂ (CO) (a c - Calculated :	amides, ureas)		Solid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	528.10 99.20 103.51	- 528.10 99.00 103.51 - 535.19 - 368.53 148.66	0.00 0.20 0.00	37HUF/FOX 60HUT/COL 60HUT/COL	
Gas phase $\Delta_i H^\circ =$	-441.16	-440.52	-0.64	88IMA/MUR	DI -2-Amino	propanoic	acid; DL-Alani	ne	C ₃ H ₇ NO ₂	
Solid phase $\Delta_t H^\circ = C_p^\circ =$	-544.21	-540.49 127.98	-3.72	88IMA/MUR	(1×C-(H (1×CO-((1×Zwitt	() ₃ (C))+(1 (C)(O))+(\times N-(H) ₂ (C)) + 1 \times O-(H)(CO) gy; aliphatic) +	(1×C-(H)(C		
						Literatu	re – Calculated =	= Residual	Reference	
(4×C-(F (2×N-(C	$C)_2(CO)) + (2$	nethylurea) ×-CH ₃ corr (q 2×CO-(N) ₂) + amides, ureas)	•	C ₇ H ₁₆ N ₄ O ₂	Gas phase $\Delta_l H^\circ =$,	-435.51			
	Literatur	e – Calculated	= Residual	Reference	Solid phase	560.50	665 DO			
Gas phase Δ _i H" =		-381.84			$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	563.58 121.71 132.21	- 557.88 121.68 132.20 - 642.81 - 366.23	-5.70 0.03 0.01	37HUF/FOX 37HUF/ELL 37HUF/ELL	
Solid phase Δ _i H° =		-546.16	- 1.54	90KAR/GUT	$\ln K_{\rm f} =$		147.73	***************************************		
(3×CO-	socyanurate (N) ₂) + (3 × ethyl cyanur	$C-(H)_3(N))+($	3×N-(C)(CC	C ₆ H ₉ N ₃ O ₃	(1×CO-(() ₃ (C)) + (1 C)(O)) + (osine ×N-(H)(C) ₂) + 1×O-(H)(CO)) gy; aliphatic)		C ₃ H ₇ NO ₂ CO)(N)) +	
(1 ~ mm		e – Calculated:	= Residual	Reference		Literatur	re – Calculated =	Residual	Reference	
Gas phase $\Delta_t H^\circ =$	-589.70	- 589.70	0.00	88IMA/MUR	Gas phase $\Delta_l H^\circ = -$	- 367.30	- 369.35	2.05	78SAB/LAF	
	.,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,				Solid phase $\Delta_t H^\circ = -$				77SAB/LAF	

TABLE 35. Amino acids (38) - Continued

TABLE 35. Amino acids (38) - Continued

$(1 \times N - (H)_2)$ $(1 \times C - (H)_2)$	oic acid (C)) + $(1 \times C - (H)_2(C)(N)$ (CO)(C)) + $(1 \times CO - (C))$ ion energy; aliphatic)	(I))+(1×C-(F (O))+(1×O	$C_4H_9NO_2$ $I)_2(C)_2) +$ -(H)(CO)) +	7-Aminoheptanoic acid $C_7H_{15}NO$ $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(C)(N)) + (4 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)) + (1 \times CO - (C)(O)) + (1 \times O - (H)(CO)) + (1 \times Zwitterion energy; aliphatic)$					
	Literature – Calculated	= Residual	Reference	Literatu	re – Calculated =	= Residual	Reference		
Gas phase				Gas phase					
$\Delta_t H^\circ =$	-443.06			$\Delta_t H^\circ =$	- 504.95				
C _p =	135.40			$C_p^{\circ} =$	204.07				
Liquid phase				Liquid phase					
$\Delta_l H^{\circ} =$	-515.35			$\Delta_{\rm f}H^{\circ} =$	- 592.54				
$C_p^{\circ} =$	235.52			$C_p^{\circ} =$	326.78				
S° =	247.34			S° = Δ _ι S° =	344.48 975.78				
$\Delta_f S^\circ = \Delta_f G^\circ =$	- 663.98 - 317.38			$\Delta_{\rm f}G^{\circ} =$	- 301.61				
$lnK_f =$	128.03			$lnK_f =$	121.67				
0-1:4				Solid phase		····			
Solid phase $\Delta_t H^\circ = -$	577.90 - 588.46	10.56	55STR/SKU2	Solid phase $\Delta_t H^\circ = -667.40$	-676.69	9.29	66SKU/BON		
$C_p^{\circ} =$	142.84	10.50	33511,5XO2	$C_p^{\circ} =$	208.60	7.25	005RO/DON		
$S^{\circ} =$	150.26			S° =	219.29				
$\Delta_t S^\circ =$	-761.06			$\Delta_{i}S^{\circ} =$	- 1100.97				
$\Delta_l G^\circ =$	-361.55			$\Delta_t G^{\circ} =$	-348.44				
	145.85			$lnK_f =$	140.56				
$InK_f = \frac{1}{(1 \times N - (H))}$ 5-Aminopenta $\frac{(1 \times N - (H))}{(1 \times C - (H))}$	nnoic acid 2(C)) + (1 × C-(H)2(C)(N	V)) + (2×C-(I	C ₅ H ₁₁ NO ₂ H) ₂ (C) ₂) + -(H)(CO)) +	9-Aminononanoic acid (1×N-(H) ₂ (C))+(1	i 1 × C−(H) ₂ (C)(N)) + (6×C-(F	$(C)_2 +$		
5-Aminopenta (1×N-(H): (1×C-(H): (1×Zwitter	nnoic acid 2(C)) + (1 × C-(H)2(C)(N 2(CO)(C)) + (1 × CO-(C) rion energy; aliphatic))(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +	9-Aminononanoic acid (1×N-(H) ₂ (C))+(1 (1×C-(H) ₂ (CO)(C) (1×Zwitterion energy)	1 1×C-(H) ₂ (C)(N)))+(1×CO-(C)(rgy; aliphatic)	(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +		
5-Aminopenta (1 × N-(H); (1 × C-(H); (1 × Zwitter	nnoic acid 2(C)) + (1 × C-(H)2(C)(N 2(CO)(C)) + (1 × CO-(C))(O))+(1×O	$(C)_2 +$	9-Aminononanoic acid (1×N-(H) ₂ (C))+(1 (1×C-(H) ₂ (CO)(C) (1×Zwitterion energy)	1 1 × C-(H) ₂ (C)(N))) + (1 × CO-(C)((O))+(1×O	C ₉ H ₁₉ NO H) ₂ (C) ₂) + -(H)(CO)) + Reference		
5-Aminopenta (1 × N-(H); (1 × C-(H); (1 × Zwitter	nnoic acid 2(C)) + (1 × C-(H)2(C)(N 2(CO)(C)) + (1 × CO-(C) rion energy; aliphatic))(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +	9-Aminononanoic acid (1×N-(H) ₂ (C))+(1 (1×C-(H) ₂ (CO)(C) (1×Zwitterion energy)	1 1×C-(H) ₂ (C)(N)))+(1×CO-(C)(rgy; aliphatic)	(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +		
5-Aminopenta (1 × N-(H); (1 × C-(H); (1 × Zwitter	nnoic acid 2(C)) + (1 × C-(H) ₂ (C)(N 2(CO)(C)) + (1 × CO-(C) 2(CO)(C)) + (1 × CO-(C) 2(CO)(C) + (1 × CO-(C) 2(C)(C) + (1 × C) 2(C)(C)(C) + (1 × C) 2(C)(C)(C)(C) + (1 × C) 2(C)(C)(C)(C) + (1 × C) 2(C)(C)(C)(C)(C) + (1 × C) 2(C)(C)(C)(C)(C)(C) + (1 × C) 2(C)(C)(C)(C)(C)(C)(C)(C) 2(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)()(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +	9-Aminononanoic acid $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C)$ $(1 \times Zwitterion eneronal distribution of the content of $	1 1×C-(H) ₂ (C)(N)))+(1×CO-(C)(rgy; aliphatic)	(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +		
5-Aminopenta (1×N-(H)): (1×C-(H)): (1×Zwitter	nnoic acid 2(C))+(1×C-(H)2(C)(N 2(CO)(C))+(1×CO-(C) rion energy; aliphatic) Literature – Calculated)(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +	9-Aminononanoic acid (1×N-(H) ₂ (C))+(i (1×C-(H) ₂ (CO)(C) (1×Zwitterion ener Literatu Gas phase	1 1 × C-(H) ₂ (C)(N))) + (1 × CO-(C)(rgy; aliphatic) rre - Calculated =	(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +		
5-Aminopenta $(1 \times N - (H))$ $(1 \times C - (H)_2$ $(1 \times Zwitter)$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase	nnoic acid 2(C)) + (1 × C-(H) ₂ (C)(N 2(CO)(C)) + (1 × CO-(C) rion energy; aliphatic) Literature – Calculated - 463.69)(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +	9-Aminononanoic acid $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C)$ $(1 \times Zwitterion eneronal distribution of the content of $	1 1 × C-(H) ₂ (C)(N) 1) + (1 × CO-(C)(0) 1 rgy; aliphatic) 1 re - Calculated = - 546.21	(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +		
5-Aminopenta $(1 \times N - (H))$ $(1 \times C - (H))$ $(1 \times Z \text{witten})$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ =$	nnoic acid 2(C)) + (1 × C-(H) ₂ (C)(N) 2(CO)(C)) + (1 × CO-(C) 1 × CO-(C))(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +	9-Aminononanoic acid $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C))$ $(1 \times Z \text{witterion energy}$ $Literatu$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ $Liquid phase$ $\Delta_t H^\circ =$	1 1 × C-(H) ₂ (C)(N) 1) + (1 × CO-(C)(rgy; aliphatic) are - Calculated = - 546.21 249.85	(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +		
5-Aminopenta $(1 \times N - (H))$: $(1 \times C - (H))$: $(1 \times Z$ witter $(1 \times Z)$ witter Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$	nnoic acid 2(C)) + (1 × C-(H) ₂ (C)(N ₂ (CO)(C)) + (1 × CO-(C)(C)) + (1 × CO-(C)(C)(C)) + (1 × CO-(C)(C)(C)) + (1 × CO-(C)(C)(C) + (1 × C)(C)(C) + (1 × C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +	9-Aminononanoic acid $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C)$ $(1 \times Z \text{witterion energy})$ Literatu Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$	1 1 × C-(H) ₂ (C)(N) 1) + (1 × CO-(C)(0) 1 rgy; aliphatic) 1 re - Calculated = -546.21 249.85 -644.00 387.62	(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +		
5-Aminopenta $(1 \times N - (H))$: $(1 \times C - (H))$: $(1 \times Z$ witter $(1 \times Z)$ witter Gas phase $\Delta_t H^\circ = C_\rho^\circ =$ Liquid phase $\Delta_t H^\circ = C_\rho^\circ =$ $C_\rho^\circ =$	nnoic acid 2(C))+(1×C-(H) ₂ (C)(N) 2(CO)(C))+(1×CO-(C) rion energy; aliphatic) Literature – Calculated - 463.69 158.29 - 541.08 265.94 279.72)(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +	9-Aminononanoic acid $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C)$ $(1 \times Z \text{witterion energy})$ Literatu Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = C_p^\circ$	1 1 × C-(H) ₂ (C)(N) 1) + (1 × CO-(C)(0) 1 rgy; aliphatic) 1 re - Calculated = - 546.21 249.85 - 644.00 387.62 409.24	(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +		
5-Aminopenta $(1 \times N - (H))$: $(1 \times C - (H))$: $(1 \times Z$ witter $(1 \times Z)$ witter Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t S^\circ =$	nnoic acid 2(C))+(1×C-(H) ₂ (C)(N) 2(CO)(C))+(1×CO-(C) rion energy; aliphatic) Literature – Calculated - 463.69 158.29 - 541.08 265.94 279.72 - 767.91)(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +	9-Aminononanoic acid $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C)$ $(1 \times Z \text{witterion energy})$ Literatu Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ $S^\circ = S^\circ = \Delta_t S^\circ =$	1 1 × C-(H) ₂ (C)(N) 1) + (1 × CO-(C)(0) 1 rgy; aliphatic) 1 re - Calculated = - 546.21 249.85 - 644.00 387.62 409.24 - 1183.64	(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +		
5-Aminopenta $(1 \times N - (H))$ $(1 \times C - (H))$ $(1 \times Z)$ $(1 \times Z)$ Gas phase $\Delta_t H^\circ = C_p^\circ = $ Liquid phase $\Delta_t H^\circ = C_p^\circ = $ $\Delta_t G^\circ = $	nnoic acid 2(C)) + (1 × C-(H) ₂ (C)(N) 2(CO)(C)) + (1 × CO-(C) rion energy; aliphatic) Literature – Calculated - 463.69 158.29 - 541.08 265.94 279.72 - 767.91 - 312.13)(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +	9-Aminononanoic acid $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C)$ $(1 \times Zwitterion energy)$ Literaturanois Base $\Delta_t H^\circ = C_p^\circ $	1 1 × C-(H) ₂ (C)(N) 1) + (1 × CO-(C)(0) 1 rgy; aliphatic) 1 re - Calculated = - 546.21 249.85 - 644.00 387.62 409.24 - 1183.64 - 291.10	(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +		
5-Aminopenta $(1 \times N - (H))$: $(1 \times C - (H))$: $(1 \times Z$ witter $(1 \times Z)$ witter Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t S^\circ =$	nnoic acid 2(C))+(1×C-(H) ₂ (C)(N) 2(CO)(C))+(1×CO-(C) rion energy; aliphatic) Literature – Calculated - 463.69 158.29 - 541.08 265.94 279.72 - 767.91)(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +	9-Aminononanoic acid $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C)$ $(1 \times Z \text{witterion energy})$ Literatu Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ $S^\circ = S^\circ = \Delta_t S^\circ =$	1 1 × C-(H) ₂ (C)(N) 1) + (1 × CO-(C)(0) 1 rgy; aliphatic) 1 re - Calculated = - 546.21 249.85 - 644.00 387.62 409.24 - 1183.64	(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +		
5-Aminopenta $(1 \times N - (H))$ $(1 \times C - (H))$ $(1 \times Z \text{ witten})$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ $Liquid phase$ $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t G^\circ = Lightarrow = Light$	- 463.69 - 541.08 - 265.94 - 267.91 - 312.13 - 312.59)(O)) + (1 × O	H ₂ (C) ₂) + -(H)(CO)) + Reference	9-Aminononanoic acide $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C))$ $(1 \times Zwitterion energy)$ Literatur Gas phase $\Delta_t H^\circ = C_\rho^\circ =$ Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ = InK_t =$ Solid phase	1 1 × C-(H) ₂ (C)(N) 1) + (1 × CO-(C)(rgy; aliphatic) 10	(O)) + (1 × O	H ₂ (C) ₂) + -(H)(CO)) + Reference		
5-Aminopenta $(1 \times N - (H))$ $(1 \times C - (H))$ $(1 \times Z \text{ witten})$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t =$ Solid phase $\Delta_t H^\circ = -$	- 463.69 - 541.08 - 265.94 - 279.72 - 767.91 - 312.13 - 312.13 - 312.87)(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +	9-Aminononanoic acid $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C))$ $(1 \times Zwitterion energy)$ Literatu Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ = InK_t =$ Solid phase $\Delta_t H^\circ = -727.80$	1 1 × C-(H) ₂ (C)(N) 1) + (1 × CO-(C)(rgy; aliphatic) 10	(O))+(1×O	H) ₂ (C) ₂) + -(H)(CO)) +		
5-Aminopenta $(1 \times N - (H))$ $(1 \times C - (H))$ $(1 \times Z \text{witter})$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t =$ Solid phase $\Delta_t H^\circ = -C_p^\circ = C_p^\circ = C_p$	- 463.69 - 541.08 - 265.94 - 279.72 - 767.91 - 604.10 - 617.87 - 15 × C-(H) ₂ (C)(N) ₂)(O)) + (1 × O	H ₂ (C) ₂) + -(H)(CO)) + Reference	9-Aminononanoic acid $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(C)) + (1 \times C - (H)_2(C)) + (1 \times C) + $	1 1×C-(H) ₂ (C)(N) 1)+(1×CO-(C)(rgy; aliphatic) 10 - Calculated = -546.21 249.85 -644.00 387.62 409.24 -1183.64 -291.10 117.43	(O)) + (1 × O	H ₂ (C) ₂) + -(H)(CO)) + Reference		
5-Aminopenta $(1 \times N - (H))$: $(1 \times C - (H))$: $(1 \times Z$ witter $(1 \times Z$ witter $(1 \times Z)$ witter Gas phase $\Delta_t H^\circ =$ $C_t^\circ =$ $\Delta_t G^\circ =$	- 463.69 - 541.08 - 265.94 - 279.72 - 767.91 - 312.13 - 312.13 - 312.73 - 312.73)(O)) + (1 × O	H ₂ (C) ₂) + -(H)(CO)) + Reference	9-Aminononanoic acid $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C)$ $(1 \times Z \text{witterion energy})$ Literatu Gas phase $\Delta_t H^\circ = C_\rho^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = 1 \text{n} K_t = S^\circ =$	1 1×C-(H) ₂ (C)(N) 1)+(1×CO-(C)(rgy; aliphatic) 1 re - Calculated = -546.21 249.85 -644.00 387.62 409.24 -1183.64 -291.10 117.43 -735.51 252.44 265.31	(O)) + (1 × O	H ₂ (C) ₂) + -(H)(CO)) + Reference		
5-Aminopenta $(1 \times N - (H))$ $(1 \times C - (H))$ $(1 \times Z \text{witter})$ Gas phase $\Delta_t H^{\circ} = C_p^{\circ} =$ Liquid phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = InK_t =$ Solid phase $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = InK_t = S^{\circ} = \Delta_t S^{\circ} = S^$	- 463.69 - 541.08 - 265.94 - 279.72 - 767.91 - 312.13 - 312.)(O)) + (1 × O	H ₂ (C) ₂) + -(H)(CO)) + Reference	9-Aminononanoic acid $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C)$ $(1 \times Z \text{witterion energy})$ Literatu Gas phase $\Delta_t H^\circ = C_\rho^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = 1 \text{n} K_t = S^\circ = S^\circ$	1 1×C-(H) ₂ (C)(N) 1)+(1×CO-(C)(rgy; aliphatic) 1	(O)) + (1 × O	H ₂ (C) ₂) + -(H)(CO)) + Reference		
5-Aminopenta $(1 \times N - (H))$: $(1 \times C - (H))$: $(1 \times Z \text{witter})$ $(1 \times Z \text{witter})$ Gas phase $\Delta_t H^\circ =$ $C_t^\circ =$ $\Delta_t H^\circ =$ $C_t^\circ =$ $\Delta_t S^\circ =$	- 463.69 - 541.08 - 265.94 - 279.72 - 767.91 - 312.13 - 312.13 - 312.73 - 312.73)(O)) + (1 × O	H ₂ (C) ₂) + -(H)(CO)) + Reference	9-Aminononanoic acid $(1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C)$ $(1 \times Z \text{witterion energy})$ Literatu Gas phase $\Delta_t H^\circ = C_\rho^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = 1 \text{n} K_t = S^\circ =$	1 1×C-(H) ₂ (C)(N) 1)+(1×CO-(C)(rgy; aliphatic) 1 re - Calculated = -546.21 249.85 -644.00 387.62 409.24 -1183.64 -291.10 117.43 -735.51 252.44 265.31	(O)) + (1 × O	H ₂ (C) ₂) + -(H)(CO)) + Reference		

L-Valine

C₅H₁₁NO₂

TABLE 35.	Amino	acids	(38)	_	Continued

TABLE 35. Amino acids (38) - Continued 2-Aminohexanoic acid; Norleucine C₆H₁₃NO₂ $(1 \times C-(H)_3(C)) + (3 \times C-(H)_2(C)_2) + (1 \times C-(H)(C)(CO)(N)) +$ $(1 \times N - (H)_2(C)) + (1 \times CO - (C)(O)) + (1 \times O - (H)(CO)) +$ (1×Zwitterion energy; aliphatic) Literature - Calculated = Residual Reference Gas phase $\Delta_f H^\circ =$ -495.14Solid phase $\Delta_t H^{\circ} =$ -639.10-643.774.67 55STR/SKU2 $C_p^{\circ} = S^{\circ} =$ 187.44 210.81 $\Delta_f S^{\circ} =$ -982.71 $\Delta_f G^{\circ} =$ -350.87 $lnK_f =$ 141.50 4-Aminohexanoic acid C₆H₁₃NO₂ $(1 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)_2(N)) +$ $(1 \times C - (H)_2(CO)(C)) + (1 \times CO - (C)(O)) + (1 \times O - (H)(CO)) +$ $(1 \times N - (H)_2(C)) + (1 \times Zwitterion energy; aliphatic)$ Literature - Calculated = Residual Reference Gas phase $\Delta_{\rm f} H^{\circ} =$ -494.35 $C_p^{\circ} =$ 179.96 Liquid phase $\Delta_{f}H^{\circ} =$ -572.54 $C_p^{\circ} =$ 300.28 *s*° = 310.64 $\Delta_f S^o =$ -873.30 $\Delta_t G^{\circ} =$ -312.16 $lnK_f =$ 125.92 Solid phase $\Delta_{\rm f}H^{\circ} =$ -646.18 -644.51-1.6755STR/SKU2 5-Aminohexanoic acid C₆H₁₃NO₂ $(1 \times C - (H)_{3}(C)) + (1 \times C - (H)(C)_{2}(N)) +$

 $(1 \times -\text{CH}_3 \text{ corr (tertiary)}) + (1 \times \text{N} - (\text{H})_2(\text{C})) + (2 \times \text{C} - (\text{H})_2(\text{C})_2) + (1 \times \text{C} - (\text{H})_2(\text{CO})(\text{C})) + (1 \times \text{CO} - (\text{C})(\text{O})) + (1 \times \text{O} - (\text{H})(\text{CO})) + (1 \times \text{O} - (\text{H})(\text{CO$

Reference

Literature - Calculated = Residual

-496.61

179.96

(1×Zwitterion energy; aliphatic)

Gas phase $\Delta_f H^\circ =$

 $C_p^{\circ} =$

	Literatur	e – Calculated =	= Residual	Reference
Gas phase				
$\Delta_{\mathbf{f}}H^{\circ} =$		-481.20		
Salid akas				
Solid phas Δ _ε H° =	e -617.90	-612.94	- 4.96	57TSU/HUN
$C_{\rho}^{\circ} =$	168.82	140.32	28.50	63HUT/COL
S° =	178.87	172.00	8.87	63HUT/COL
$\Delta_f S^{\circ} =$	_,_,	-875.63		
$\Delta_f G^\circ =$		-351.87		
$lnK_f =$		141.94		
(1×C-((1×CO	$(H)_3(C) + (1)_3(C)_2 + (1)_2(C)_2 + (1)_2(C)(O) + (1)_3(C)_3 + (1)_$	×C-(H)(C) ₃)+ 1×C-(H)(C)(C 1×O-(H)(CO) gy; aliphatic)	O)(N))+(1×)+	N−(H) ₂ (C))+
	Literatui	re – Calculated	= Residuai	Reference
Gas phase				
$\Delta_i H^{\circ} =$		- 501.83		
Solid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	- 640.60 194.30 207.10	-642.35 162.24 195.01 -988.93 -347.50 140.18	1.75 32.06 12.09	37HUF/FOX 37HUF/ELL 37HUF/ELL
$lnK_f =$				
DL-Isoleu (1 × O-((1 × N-((1 × C-($(H)(CO) + (H)_2(C) + (I)_2(C)_2 + (I)_2(C)$	$(1 \times CO - (C)(O))$ $\times C - (H)(C)_3) + (2 \times C - (H)_3(C))$ $(2 \times C)_3 = (1)$	+ (1 × -CH ₃ co +	
DL-Isoleu (1 × O-((1 × N-((1 × C-($(H)(CO) + (H)_2(C) + (I)_2(C)_2 + (I)_2(C)$	\times C-(H)(C) ₃) $+$ 2 \times C-(H) ₃ (C)) gy; aliphatic)	+ (1 × -CH ₃ co +	(C)(CO)(N))+
DL-Isoleu (1 × O-((1 × N-((1 × C-((H)(CO)) + (1 (H) ₂ (C)) + (1 (H) ₂ (C) ₂) + (2 itterion ener	\times C-(H)(C) ₃) $+$ 2 \times C-(H) ₃ (C)) gy; aliphatic)	+ (1 × -CH ₃ co +	(C)(CO)(N))+ rr (tertiary))+

ESTIMATION OF THERMODYNAMIC PROPERTIES OF ORGANIC COMPOUNDS

TABLE 35. Amino acids (38) - Continued

TABLE 35. Amino acids (38) - Continued

5-Aminohexanoic acid (Continued) C_6H $(1 \times C - (H)_3(C)) + (1 \times C - (H)(C)_2(N)) +$ $(1 \times - CH_3 \text{ corr (tertiary)}) + (1 \times N - (H)_2(C)) + (2 \times C - (H)_2(C)_2(1 \times C - (H)_2(CO)(C)) + (1 \times CO - (C)(O)) + (1 \times O - (H)(CO)) +$ $(1 \times Z \text{ witterion energy; aliphatic})$	13NO ₂ DL-Ornithine $C_5H_{12}N_2O_2$ $(1 \times N - (H)_2(C) \text{ (second, amino acids)}) + (1 \times C - (H)_2(C)(N)) +$ $(2 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)(CO)(N)) + (1 \times N - (H)_2(C)) +$ $(1 \times CO - (C)(O)) + (1 \times O - (H)(CO)) +$ $(1 \times Z\text{witterion energy; aliphatic)}$
Literature - Calculated = Residual Reference	e Literature – Calculated = Residual Reference
Liquid phase $\Delta_t H^\circ = -574.72$ $C_s^\circ = 300.28$	Gas phase $\Delta_t H^\circ = -441.30$
$C_p^{\circ} = 300.28$ $S^{\circ} = 310.64$ $\Delta_k S^{\circ} = -873.30$	Solid phase
$\Delta_t G^\circ = -314.34$ $\ln K_t - 126.80$	$\Delta_t H^\circ = -652.60 -647.62 -4.98$ 60PON/MIG $C_p^\circ = 191.33 191.26 0.07$ 40HUF/FOX $S^\circ = 193.30 193.29 0.01$ 40HUF/FOX $\Delta_t S^\circ = -1015.38$
Solid phase Δ _t H° = -643.29 -646.85 3.56 55STR/S	$\Delta_t G^{\circ} = -344.88$
DL-Serine; 3-Hydroxy-2-aminopropanoic acid (1×O-(H)(CO))+(1×CO-(C)(O))+(1×C-(H)(C)(CO)(N) (1×N-(H) ₂ (C))+(1×C-(H) ₂ (O)(C))+(1×O-(H)(C))+ (1×Zwitterion energy; aliphatic)	H ₇ NO ₅ DL-Lysine $C_6H_{14}N_2O_2$)+ $(1 \times O - (H)(CO)) + (1 \times CO - (C)(O)) + (1 \times N - (H)_2(C)) +$ $(1 \times C - (H)(C)(CO)(N)) + (3 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)(N)) +$ $(1 \times N - (H)_2(C) \text{ (second, amino acids)}) +$ $(1 \times Z\text{witterion energy; aliphatic)}$
Literature - Calculated = Residual Reference	
Gas phase $\Delta_t H^\circ = -583.22$	Gas phase $\Delta_t H^\circ = -461.93$
Solid phase $ \Delta_t H^\circ = -732.70 -737.96 \qquad 5.26 \qquad 78SAB/L \\ C_\rho^\circ = 132.21 \qquad 105.40 \qquad 26.81 \qquad 75SPI/W. \\ S^\circ = \qquad \qquad 128.86 \\ \Delta_t S^\circ = \qquad \qquad -748.67 \\ \Delta_t G^\circ = \qquad \qquad -514.74 \\ \ln K_\ell = \qquad 207.64 $	•
3-Hydroxy-2-aminobutanoic acid; DL-Threonine C_4 $(1 \times C-(H)_3(C)) + (1 \times C-(H)(O)(C)_2 \text{ (alcohols, peroxides)}) + (1 \times -CH_3 \text{ corr (tertiary)}) + (1 \times O-(H)(C)) + (1 \times C-(H)(C)(CO)(N)) + (1 \times N-(H)_2(C)) + (1 \times CO-(C)(O)) + (1 \times O-(H)(CO)) + (1 \times Z\text{witterion energy; aliphatic})$	H ₂ NO ₃ L-Aspartic acid $(2 \times O - (H)(CO)) + (2 \times CO - (C)(O)) + (1 \times C - (H)(C)(CO)(N)) + (1 \times N - (H)_2(C)) + (1 \times C - (H)_2(CO)(C)) + (1 \times Zwitterion energy; aliphatic)$
Literature - Calculated = Residual Reference	e Literature – Calculated = Residual Reference
Gas phase $\Delta_i H^{\circ} = -620.94$	Gas phase $\Delta_t H^\circ = -804.37$
Solid phase $\Delta_t H^\circ = -758.80 -786.62$ 27.82 60POM/S $C_p^\circ = 155.70$ $S^\circ = 167.77$ $\Delta_t S^\circ = -846.07$ $\Delta_t G^\circ = -534.36$ $\ln K_t = 215.56$	Solid phase $\Delta_{\rm f}H^{\circ} = -973.28 -972.45 -0.83 36 {\rm HUF/ELL}$ $C_{\rho}^{\circ} = 155.18 165.73 -10.55 63 {\rm HUT/COL2}$ $S^{\circ} = 170.12 154.15 15.97 63 {\rm HUT/COL2}$ $\Delta_{\rm f}S^{\circ} = -831.64$ $\Delta_{\rm f}G^{\circ} = -724.50$ $\ln K_{\rm f} = 292.26$

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TABLE 35. Amino acids (38) - Continued

TABLE 35.	Amino	acids (38	3) —	Continued
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(1×C-(H	acid I)(CO))+(2×CO-(C)(O))- ()(C)(CO)(N))+(1×N-(H): erion energy; aliphatic)+(1	₂ (C))+		(1×C-(H	H)(C _B) ₂)+ I)(C)(CO)((1×C _B -(C)(C _E N))+(1×N-(I 1×Zwitterion	$H)_2(C)) + (1 \times$	CO-(C)(O))+
	Literature - Calculated =	Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas phase Δ _t H° =	-825.00	·		Gas phase Δ _t H° =		-319.64		
Solid phase $\Delta_t H^\circ = -1$ $C_t^\circ = S^\circ = $ $\Delta_t S^\circ = $ $\Delta_t G^\circ = $ $\ln K_t = $		-7.84 -12.59 11.04	52TSU/HUN 63HUT/COL2 63HUT/COL2	Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 459.80 203.01 213.64	-461.25 205.00 211.06 -859.53 -203.98 82.28	1.45 - 1.99 2.58	52BRE/DER 63COL/HUT 63COL/HUT
(1 × C-(H (1 × N-(H	ne H)(CO)) + (1 × CO-(C)(O)) H) ₂ (CO)(C)) + (1 × CO-(C)(1 H) ₂ (CO) (amino acids)) + (1 terion energy; aliphatic)	N))+		$(1 \times C_{B} - (C_{B} - (C_{B}$	$C)(C_B)_2) + (I)_2(C)) + (1$	\times C _B -(O)(C _B): $1 \times$ C-(H) ₂ (C)(\times CO-(C)(O)) gy, aromatic I)	(C_B)) + (1 × C- + (1 × O-(H))	(H)(C)(CO)(N)) +
	Literature - Calculated =	Residual	Reference		Literatui	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ =$	- 609.09			Gas phase Δ _l H° =		- 498.50		
Solid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	7788.70 — 791.05 159.80 161.03 174.50 173.27 — 843.62 — 539.53 217.64	2.35 -1.23 1.23	36HUF/ELL 32HUF/BOR 32HUF/BOR	Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 685.10 216.44 214.01	666.03 213.83 218.52 954.59 381.42 153.86	~ 19.07 2.61 - 4.51	37HUF/FOX 63COL/HUT 63COL/HUT
(1 × C-(1 (1 × N-(1	ne H)(CO)) + (1 × CO-(C)(O)) H) ₂ (CO)(C)) + (1 × C-(H) ₂ (C H) ₂ (CO) (amino acids)) + (1 tterion energy; aliphatic)	$(1 \times C)_2$	O-(C)(N))+	(1 × O-(H (1 × Zwitt	H)(C _B) ₂) + I)(CO)) + ($(1 \times N - (H)_{2}(C_{E}) \times CO - (O)(C_{E})$ $(1 \times CO - (O)(C_{E}) \times (O)$ $(1 \times N - (O)(C_{E}))$	$(1 \times C_{B} - (1 \times C_{B}))$	
	Literature - Calculated =	Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_i H^{\circ} =$	- 629.72			Gas phase $\Delta_t H^\circ =$	- 296.00	290.61	-5.39	74SAB/CHA
Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ - \Delta_t G^\circ =$	-825.50 -820.46 184.18 182.98 195.06 196.28 -956.92 -535.15	-5.04 1.20 -1.22	57TSU/HUN 63HUT/COL2 63HUT/COL2	Liquid phas $\Delta_t H^\circ = C_p^\circ =$	e 380.40	-380.00 258.70	- 0.40	71LEB/GUT

TABLE 35. Amino acids (38) - Continued

TABLE 35. Amino acids (38) - Continued

$ \begin{array}{ll} \textbf{2-Aminobenzoic acid (Continued)} & C_7H_7NO_2\\ (4\times C_B-(H)(C_B)_2)+(1\times N-(H)_2(C_B))+(1\times C_B-(N)(C_B)_2)+\\ (1\times O-(H)(CO))+(1\times CO-(O)(C_B))+(1\times C_B-(CO)(C_B)_2)+\\ (1\times Zwitterion energy, aromatic II)+\\ (1\times NH_2-COOH\ (ortho\ corr)) \end{array} $	$ \begin{array}{ll} \textbf{2-Aminobenzoic acid (Continued)} & \textbf{C}_7H_7NO_2\\ (4 \times C_{B^-}(H)(C_B)_2) + (1 \times N(H)_2(C_B)) + (1 \times C_{B^-}(N)(C_B)_2) + \\ (1 \times O(H)(CO)) + (1 \times CO(O)(C_B)) + (1 \times C_{B^-}(CO)(C_B)_2) + \\ (1 \times Zwitterion energy, aromatic II) + \\ (1 \times NH_2\text{-COOH (ortho corr))} \end{array} $
Literature - Calculated = Residual Reference	Literature - Calculated = Residual Reference
Solid phase $\Delta_t H^\circ = -400.90 -401.73 0.83 71 LEB/GUT$ $C_\rho^\circ = 165.27 165.27 0.00 26 AND/LYN$ $S^\circ = 168.42$ $\Delta_t S^\circ = -629.55$ $\Delta_t G^\circ = -214.03$ $\ln K_f = 86.34$	Solid phase $\Delta_{t}H^{\circ} = -412.80 -415.73 2.93 77NAB/SAB$ $C^{\circ}_{\rho} = 177.82 169.98 7.84 26AND/LYN$ $S^{\circ} = 168.42$ $\Delta_{t}S^{\circ} = -629.55$ $\Delta_{t}G^{\circ} = -228.03$ $\ln K_{t} 91.99$
3-Aminobenzoic acid $C_7H_7NO_2$ $(4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (N)(C_B)_2) + (1 \times N - (H)_2(C_B)) + (1 \times C_B - (CO)(C_B)_2) + (1 \times CO - (O)(C_B)) + (1 \times O - (H)(CO)) + (1 \times Zwitterion energy, aromatic II) + (1 \times NH_2 - COOH (meta~corr))$	N-Phenylglycine $(5\times C_B-(H)(C_B)_2)+(1\times C_B-(N)(C_B)_2)+(1\times N-(H)(C)(C_B))+\\ (1\times C-(H)_2(CO)(N))+(1\times CO-(C)(O))+(1\times O-(H)(CO))+\\ (1\times Zwitterion\ energy,\ aromatic\ II)$ Literature – Calculated = Residual Reference
Literature - Calculated = Residual Reference	· · · · · · · · · · · · · · · · · · ·
Gas phase $\Delta_t H^\circ = -283.60 -290.61$ 7.01 74SAB/CHA	Gas phase $\Delta_t H^\circ = -267.89$
Liquid phase $\Delta_t H^\circ = -389.80 -390.00$ 0.20 71LEB/GUT $C_p^\circ = 258.70$	Solid phase $\Delta_t H^\circ = -402.50 -398.75 -3.75$ 04FIS/WRE $C_p^\circ = 176.60$ 180.15 -3.55 80SAB/SKO
Solid phase $ \Delta_t H^\circ = -410.70 \qquad -411.73 \qquad 1.03 \qquad 71 LEB/GUT $ $ C_p^\circ = 162.76 \qquad 162.76 \qquad 0.00 \qquad 26 AND/LYN $ $ S^\circ = \qquad 168.42 \qquad \qquad$	Hippuric acid; N-Benzoylglycine $C_9H_9NO_2$ $(5 \times C_B - (H)(C_B)_2) + (1 \times C_B - (CO)(C_B)_2) + (1 \times CO - (C_B)(N)) +$ $(1 \times N - (H)(C)(CO) \text{ (amino acids)}) + (1 \times C - (H)_2(CO)(N)) +$ $(1 \times CO - (C)(O)) + (1 \times O - (H)(CO)) +$ $(1 \times Z \text{ witterion energy, aromatic II)}$ Literature-Calculated = Residual Reference
	Solid phase $\Delta_t H^\circ = -608.90 -609.15 0.25$ 61HUB/FRO $C_p^\circ = 214.35$ 214.56 -0.21 41HUF
Literature - Calculated = Residual Reference	Glycylglycine $C_4H_8N_2O_3$ $(1 \times N - (H)_2(C)) + (2 \times C - (H)_2(CO)(N)) + (1 \times CO - (C)(N)) +$
Gas phase $\Delta_t H^{\circ} = -296.70 - 290.61 - 6.09$ 74SAB/CHA	$(1 \times N - (H)(C)(CO) \text{ (amino acids)}) + (1 \times CO - (C)(O)) + (1 \times O - (H)(CO)) + (1 \times Zwitterion energy; aliphatic)$ Literature – Calculated = Residual Reference
Liquid phase $\Delta_t H^\circ = -391.90 -392.00$ 0.10 71LEB/GUT $C_\rho^\circ = 258.70$	Gas phase $\Delta_t H^\circ = -528.03$
	Solid phase $\Delta_t H^\circ = -747.68 -748.15$ 0.17 92DIA/DOM $C_p^\circ = 163.97$ 163.22 0.75 69HUT/COL2

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TABLE 35. Amino acids (38) — Continued	TABLE 35. Amino acids (38) — Continued					
DL-Alanylglycine $C_5H_{10}N_2O_3$ $(1 \times N-(H)_2(C)) + (1 \times C-(H)(C)(CO)(N)) + (1 \times C-(H)_3(C)) +$ $(1 \times -CH_3 \text{ corr (tertiary)}) + (1 \times CO-(C)(N)) +$ $(1 \times N-(H)(C)(CO) \text{ (amino acids)}) + (1 \times C-(H)_2(CO)(N)) +$ $(1 \times CO-(C)(O)) + (1 \times O-(H)(CO)) +$ $(1 \times Z\text{witterion energy; aliphatic)}$	N-Glycyl-DL-valine ${}^{7}H_{14}N_{2}C$ $(1 \times N - (H)_{2}(C)) + (1 \times C - (H)_{2}(CO)(N)) + (1 \times CO - (C)(N + (1 \times N - (H)(C)(CO) + (1 \times C - (H)(C)(CO) + (1 \times C - (H)(C)(CO)) + (1 \times C - (H)(C)(CO)) + (1 \times C - (H)_{3}(C)) + (2 \times $					
Literature - Calculated = Residual Reference	Literature - Calculated = Residual Ref :nce					
Gas phase $\Delta_t H^\circ = -588.15$	Gas phase $\Delta_t H^\circ = -633.84$					
Solid phase $\Delta_t H^\circ = -777.80 -777.93 0.13 42 \text{HUF}$ $C_p^\circ = 182.83 185.90 -3.07 41 \text{HUF}$	Solid phase $\Delta_t H^\circ = -835.00 -832.99 -2.01$ 62Pt J/ALE $C_p^\circ = 204.54$					
$\begin{array}{ll} \textbf{DL-Alanyl-DL-alanine} & C_6H_{12}N_2O_3 \\ (1\times N-(H)_2(C)) + (2\times C-(H)_3(C)) + (2\times -CH_3 \text{ corr (tertiary)}) + \\ (2\times C-(H)(C)(CO)(N)) + (1\times CO-(C)(N)) + \\ (1\times N-(H)(C)(CO) \text{ (amino acids)}) + (1\times CO-(C)(O)) + \\ (1\times O-(H)(CO)) + (1\times Z \text{witterion energy; aliphatic)} \end{array}$	$ \begin{array}{lll} \mbox{Hippurylglycine} & (-B_{12}N_2O) \\ (5 \times C_B - (H)(C_B)_2) + (1 \times C_B - (CO)(C_B)_2) + (1 \times CO - (C_B)(1 - 1) + \\ (2 \times N - (H)(C)(CO) & (amino acids)) + (2 \times C - (H)_2(CO)(N - 1) + \\ (1 \times CO - (C)(N)) + (1 \times CO - (C)(O)) + (1 \times O - (H)(CO)) + \\ (1 \times Zwitterion energy, aromatic II) \end{array} $					
Literature - Calculated = Residual Reference	Literature-Calculated = Residual Reference					
Gas phase $\Delta_t H^\circ = -648.27$	Solid phase $\Delta_t H^\circ = -832.00 -829.20 -2.80$ 42HUF $C_p^\circ = 278.00$ 278.78 -0.78 41HUF					
Solid phase $\Delta_l H^\circ = -807.32 - 807.71 0.39$ 92DIA/DOM $C_p^\circ = 208.58$	Glycylphenylalanine $C_{11}H_{14}N_2O$ $(1\times N-(H)_2(C))+(1\times C-(H)_2(CO)(N))+(1\times CO-(C)(N))+$					
$\begin{array}{ll} \textbf{DL-Leucylglycine} & C_{8}H_{16}N_{2}O_{3} \\ (2\times C-(H)_{3}(C)) + (1\times C-(H)(C)_{3}) + (1\times -CH_{3} \text{ corr (tertiary)}) + \\ (1\times C-(H)_{2}(C)_{2}) + (1\times N-(H)_{2}(C)) + (1\times C-(H)(C)(CO)(N)) + \\ (1\times CO-(C)(N)) + (1\times N-(H)(C)(CO) \text{ (amino acids)}) + \\ (1\times C-(H)_{2}(CO)(N)) + (1\times CO-(C)(O)) + (1\times O-(H)(CO)) + \\ (1\times C-(H)_{2}(CO)(N)) + (1\times CO-(C)(O)) + (1\times O-(H)(CO)) + \\ (1\times C-(H)_{2}(CO)(N)) + (1\times CO-(C)(O)) + (1\times O-(H)(CO)) + \\ (1\times C-(H)_{2}(CO)(N)) + (1\times CO-(C)(O)) + (1\times O-(H)(CO)) + \\ (1\times C-(H)_{2}(CO)(N)) + (1\times C-(H)(CO)(N)) + (1\times C-(H)(CO)(N)) + \\ (1\times C-(H)_{2}(CO)(N)) + (1\times C-(H)(C)(O)(N)) + (1\times C-(H)(CO)(N)) + \\ (1\times C-(H)_{2}(CO)(N)) + (1\times C-(H)(C)(O)(N)) + (1\times C-(H)(C)(O)(N)) + \\ (1\times C-(H)_{2}(CO)(N)) + (1\times C-(H)(C)(O)(N)) + (1\times C-(H)(C)(O)(N)) + \\ (1\times C-(H)_{2}(CO)(N)) + (1\times C-(H)(C)(O)(N)) + (1\times C-(H)(C)(O)(N)) + \\ (1\times C-(H)_{2}(CO)(N)) + (1\times C-(H)(C)(O)(N)) + (1\times C-(H)(C)(O)(N)) + \\ (1\times C-(H)_{2}(CO)(N)) + (1\times C-(H)(C)(O)(N)) + (1\times C-(H)(C)(O)(N)) + \\ (1\times C-(H)_{2}(CO)(N)) + (1\times C-(H)(C)(O)(N)) + (1\times C-(H)(C)(O)(N)) + (1\times C-(H)(C)(O)(N)) + \\ (1\times C-(H)_{2}(CO)(N)) + (1\times C-(H)(C)(O)(N)(N) + (1\times C-(H)(C)(O)(N)(N)) + (1\times C-(H)(C)(O)(N)(N)(N)(N)(N)(N)(N)(N)(N)(N)(N)(N)(N)$	$(1\times N-(H)(C)(CO) \text{ (amino acids)}) + (1\times C-(H)(C)(CO)(N)) + \\ (1\times C-(H)_2(C)(C_B)) + (5\times C_B-(H)(C_B)_2) + (1\times C_B-(C)(C_B)_2) + \\ (1\times CO-(C)(O)) + (1\times O-(H)(CO)) + \\ (1\times Zwitterion energy, aromatic I)$ $Literature - Calculated = Residual \qquad Reference$					
(1 × Zwitterion energy; aliphatic) Literature – Calculated = Residual Reference	Gas phase $\Delta_t H^\circ = -472.28$					
Gas phase $\Delta_t H^\circ = -652.21$	Solid phase $\Delta_t H^\circ = -684.50 -681.30 -3.20$ 62PON/ALE $C^\circ_\rho = 269.22$					
Solid phase $\Delta_i H^\circ = -859.80 - 860.06$ 0.26 42HUF $C_p^\circ = 256.34$ 226.46 29.88 41HUF						

TABLE 35. Amino acids (38) - Continued

TABLE 36. Nitroso (9)

$(1 \times -CH_3)$ $(1 \times N - (H))$ $(5 \times C_B - (H))$	lalanine $(2)(C) + (2 \times C - (H)(C)(CO)(N)) + (1 \times CO - (C)(N)) + (1 \times CO - (C)(N)) + (1 \times CO - (C)(N)) + (1 \times C - (H)(C_B)_2) + (1 \times C_B - (C)(C_B)_2) + (1 \times CO)(CO)) + (1 \times Zwitterion energy, arongonical contents)$) ₂ (C)(C _B)) + O-(C)(O)) +	Dimethylnitrosoamine $C_2H_6N_2$ ($2 \times C - (H)_3(N)) + (2 \times -CH_3 \text{ corr (quaternary)}) + (1 \times N - (C)_2(NO))$ Literature – Calculated = Residual Reference
	Literature – Calculated = Residual	Reference	Gas phase $\Delta_t H^\circ = -3.30 -3.64 0.34 67 \text{KOR/PEP}$
Gas phase $\Delta_t H^\circ =$	-532.40		Liquid phase $\Delta_t H^{\circ} = -44.80 - 45.00 0.20 67 \text{KOR/PEP}$
Solid phase $\Delta_t H^\circ = C_p^\circ =$	-710.40 -711.08 0.68 291.90	62PON/ALE	Nitrosobenzene $C_6N_5N_6$ (5 × C_B -(H)(C_B) ₂) + (1 × C_B -(NO)(C_B) ₂)
			Literature - Calculated = Residual Reference
(1×N-(H (2×N-(H (1×C-(H (1×O-(H	phenylalanine) ₂ (C)) + $(1 \times C - (H)_2(CO)(N)) + (2 \times C)(C)(CO)$ (amino acids)) + $(2 \times C - (H)_3(C)) + (1 \times - CH_3 \text{ corr (tertiary)}) + (1 \times C - (H)_2(C)(C_B)) + (5 \times C)(C_B)$	$(C)(CO)(N)) + 1 \times CO - (C)(O)) + C_B - (H)(C_B)_2) +$	Gas phase $\Delta_t H^\circ = 90.55$
(1×C _B −(€	$C(C_B)_2 + (1 \times Zwitterion energy, aro$ $Literature - Calculated = Residual$	Reference	Solid phase $\Delta_t H^{\circ} = -30.00$ 55.65 -85.65 30DRU/FLA
Gas phase Δ _t H° =	-685.04		N-Nitrosopiperidine $C_5H_{10}N_2C_3$ $(3\times C-(H)_2(C)_2)+(2\times C-(H)_2(C)(N))+(1\times N-(C)_2(NO))+(1\times N-Nitrosopiperidine rsc)$
Solid phase $\Delta_t H^\circ = C_p^\circ =$	- 926.80 - 931.13 4.33 356.12	62PON/ALE	Literature – Calculated = Residual Reference
Valylphenyl	alanine	C ₁₄ H ₂₀ N ₂ O ₃	Gas phase $\Delta_t H^{\circ} = 16.60$ 16.71 -0.11 74GOL/PEP
$(1 \times C - (H + C))))))))))))))))))$	$(1)_2(C)$) + $(2 \times C - (H)(C)(CO)(N))$ + $(2 \times C - (H)(C)(CO)(N))$ + $(2 \times C)$ + $(1 \times - CH_3 \text{ corr (tertiary)})$ + $(1 \times C)$ + $(1 \times $	1 × CO-(C)(N)) +) ₂ (C)(C _B)) + O-(C)(O)) +	Liquid phase $\Delta_t H^\circ = -31.10$ -31.09 -0.01 74GOL/PEP
	Literature – Calculated = Residual	Reference	4-Nitroso-1-naphthol $C_{10}H_7NO_1$ $(6 \times C_B-(H)(C_B)_2) + (2 \times C_BF-(C_BF)(C_B)_2) + (1 \times C_B-(O)) +$
Gas phase $\Delta_l H^\circ =$	- 575.83		$(1 \times \text{naphthalene 2 sub}) + (1 \times O - (H)(C_B)) + (1 \times C_B - (NO))$ Literature - Calculated = Residual Reference
Solid phase $\Delta_t H^\circ = C_p^\circ =$	-766.10 -763.80 -2.30 310.54	63PON/ALE	Gas phase $\Delta_t H^{\circ} = -20.50 -20.49 -0.01$ 68HAM/FAG
	· · · · · · · · · · · · · · · · · · ·		Solid phase $\Delta_t H^\circ = -107.90 -107.87 -0.03$ 68HAM/FAG

TABLE 36. Nitroso (9) - Continued

TABLE 37. Nitro compounds (50)

		trinitrosamine; ×N-(C) ₂ (NO)		C ₃ H ₆ N ₆ O ₆ rsc)	Nitrometha (1×C-(H		Nitromethane),	$\sigma = 3$	CH₃NO
	Literat	ture-Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
1,5-Dinitroso 3,7-Dinitroso (5 × C-(H)	-1,3,5,7-tet $p_2(N)_2) + (2$	282.30 ylenetetramine raazabicyclo[3. × N-(C) ₃) + (2	3.1]nonane	49MED/THO C ₅ H ₁₀ N ₆ O ₂	Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	-74.86 57.32 275.01	-74.86 57.32 275.01 -227.38 -7.07 2.85	0.00 0.00 0.00	54MCC/SCO 69STU/WES 69STU/WES
(1×DINO		ture-Calculated	= Residual	Reference	$C_p^{\circ} =$	-112.60 105.98	-112.60 105.98	0.00 0.00	73LEB/RYA 47JON/GIA
Solid phase Δ _t H° =	228.70	228.70	0.00	56MED/THO	$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f =$	171.75	171.75 -330.64 -14.02 5.66	0.00	47JON/GIA
)₃(C))+(2: C))+(1× <i>N</i>	exide \times C-(H) ₂ (C) ₂) + \times (oxide)(C)) \times - Calculated =		$C_4H_{14}N_2O$ $C)(N_A)) +$ Reference	Dinitrometh (1×C-(H	I) ₂ (NO ₂) ₂ ,	Dinitromethane	,	CH ₂ N ₂ O. Reference
Gas phase $\Delta_t H^\circ =$	-31.00	- 16.88	- 14.12	81BYS	Gas phase $\Delta_t H^\circ =$	- 58.90	- 58.90	0.00	71KNO/MIR
Liquid phase Δ _t H° =	- 82.70	- 70.58	- 12.12	81BYS	Liquid phas $\Delta_l H^\circ =$	e - 104.90	- 104.90	0.00	71KNO/MIR
) ₃ (C)) + (2 oxide)(C)) -	oxide × C-(C)3(N _A)) + (6×-CH3 cor e Calculated =	r (quaternary		Trinitromet	I)(NO ₂) ₃ , 7	Frinitromethane	•	CHN ₃ O ₄
Gas phase $\Delta_t H^\circ = -$	- 107.60	-107.62	0.02	81BYS	Gas phase Δ _t H° =	-0.30	- 0.30	0.00	67MIR/LEB
Liquid phase $\Delta_t H^\circ = -$		-153.50	0.00	81BYS	Liquid phas $\Delta_t H^\circ =$	e -32.80	-32.80	0.00	67MIR/LEB
N-oxide	·	1,4-Dicyanoben (2×C _B -(CNO))		C ₈ H ₄ N ₂ O ₂	Solid phase $\Delta_t H^{\circ} =$	-48.00	-48.00	0.00	67MIR/LEB
	Literatur	e - Calculated =	= Residual	Reference	Tetranitrom (1×C-(N		anitromethane)		CN₄O₀
Gas phase Δ _t H° =	410.50	410.50	0.00	92ACR/TUC		Literatu	re – Calculated =	= Residual	Reference
Solid phase Δ _t H° =	337.50	337.50	0.00	92ACR/TUC	Gas phase $\Delta_t H^\circ =$	82.30	82.30	0.00	75LEB/MIR

ESTIMATION OF THERMODYNAMIC PROPERTIES OF ORGANIC COMPOUNDS

TABLE 37. Nitro compounds (50) - Continued

	ABLE 37. I	itro compound	is (30) — Co			TABLE 57.	====	IS (30) — CI	
Fetranitrom (1 × C-(N		ntinued) mitromethane)		CN ₄ O ₈		ane (Contin H)3(C))+(2		+ (1 × C-(H) ₂	$C_4H_9NO_2$ (C)(NO ₂)), $\sigma = 6$
	Literatur	e – Calculated =	= Residual	Reference		Literatu	re – Calculated :	= Residual	Reference
Liquid phas Δ _t H° =	e 38.30	38.30	0.00	75LEB/MIR	Liquid pha $ \Delta_t H^\circ = C_\rho^\circ = $	nse – 192.51	- 192.57 195.06	0.06	49HOL/DOR
Nitroethane (1×C-(H		×C-(H)₂(C)(N	O_2)), $\sigma = 6$	C ₂ H ₅ NO ₂	1-Nitropen (1×C-(1		×C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂	$C_5H_{11}NO_2$ (C)(NO ₂)), $\sigma = 6$
	Literatur	e – Calculated =	= Residual	Reference		Literatu	re – Calculated :	= Residual	Reference
Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	- 102.30 78.20 315.43	-102.76 78.87 316.02 -322.68 -6.55 2.64	0.46 - 0.67 - 0.59	49HOL/DOR 69STU/WES 69STU/WES	Gas phase $ \Delta_t H^\circ = C_r^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $		- 164.65 147.54 433.50 - 614.13 18.45 - 7.44		
Liquid phas $\Delta_t H^\circ = C_p^\circ =$	se 143.90 134.22	-141.11 134.22	-2.79 0.00	73LEB/RYA 66LIU/ZIE	Liquid pha $\Delta_t H^\circ = C_p^\circ =$		-218.30 225.48	2.90	73LEB/RYA
1-Nitroprop (1×C-(F		× C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂ ($C_3H_7NO_2$ $(C)(NO_2)), \sigma = 6$		$H)_3(C)) + (1$	\times C-(H)(C) ₂ (N iary)), $\sigma = 18$	O ₂))+	C ₃ H ₇ NO ₃
	Literatu	re – Calculated	= Residual	Reference		Literatu	re – Calculated =	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f =$	- 123.80 102.13 355.64	- 123.39 101.76 355.18 - 419.83 1.78 - 0.72	-0.41 0.37 0.46	49HOL/DOR 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	- 139.00 101.50 347.69	- 142.04 101.04 345.93 - 429.08 - 14.11 5.69	3.04 0.46 1.76	49HOL/DOR 69STU/WES 69STU/WES
Liquid phas $ \Delta_t H^\circ = C_p^\circ = $	se 167.20	-166.84 164.64	-0.36	73LEB/RYA	Liquid pha $\Delta_t H^\circ =$	se -180.30	- 182.08	1.78	58CAS/FLE
1-Nitrobuta (1×C-(F		×C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂ ($C_4H_9NO_2$ (C)(NO ₂)), $\sigma = 6$		$H)_2(C)_2) + (2$	$2 \times C - (H)_3(C)$ Hary)), $\sigma = 18$	+ (1 × C-(H)((C4H•NO2 C)2(NO2))+
	Literatu	re – Calculated	= Residual	Reference		Literatu	re – Calculated =	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_f = $	-143.90 124.89 394.47	- 144.02 124.65 394.34 - 516.98 10.12 - 4.08	0.12 0.24 0.13	49HOL/DOR 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_f =$	-163.60 123.47 383.34	- 160.41 123.93 385.09 - 526.23 - 3.51 1.42	-3.19 -0.46 -1.75	49HOL/DOR 69STU/WES 69STU/WES

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TABLE 37. Nitro compounds (50) -	- Continued
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1,1-Dinitrop (1 × C–(H	entane I)3(C))+(3	× C-(H) ₂ (C) ₂)	+ (1×C-(H)(C ₅ H ₁₀ N ₂ O ₂ C)(NO ₂) ₂)
	Literatur	re – Calculated	= Residual	Reference
Gas phase Δ ₁ H° –		140.95		
Liquid phas $\Delta_t H^\circ =$		-213.60	-3.30	68LEB/RYA2
1,2-Dinitroe (2×C-(H))+(1×NO _z -1	NO2 (corr, ali	C₂H₄N₂O , oh, adjacent))
	Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_l H^\circ = C_p =$		-101.00 106.28		
Liquid phas $\Delta_t H^\circ = C_p^\circ =$		167.00 195.48	1.80	68LEB/RYA2
Solid phase Δ _i H° =		- 178.00	-0.80	68LEB/RYA2
1,3-Dinitrop (1 × C-(H		2×C-(H)₂(C)(l	NO ₂))	C ₃ H ₆ N ₂ O ₄
	Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$		- 141.63 129.17		
Liquid phas $\Delta_t H^\circ = C_p^\circ =$	e 215.50	-212.73 225.90	- 2.77	71LEB/GUT
1,4-Dinitrob		2×C-(H)₂(C)(1	NO ₂))	C ₄ H ₈ N ₂ O ₄
, (e – Calculated		Reference

2-Nitrobutane (Continued) $(1 \times C - (H)_2(C)_2) + (2 \times C - (H)_3(C)) + (1 \times C - (H))(1 \times - CH_3) = 18$	C ₄ H ₉ NO ₂ (C) ₂ (NO ₂)) +	1,1-Dinitropentane $(1 \times C - (H)_3(C)) + (3 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)_2(C)_2)$
Literature – Calculated = Residual	Reference	Literature – Calculated = Residual
Liquid phase $\Delta_t H^\circ = -207.50 -205.63 -1.87$	49HOL/DOR	Gas phase Δ ₁ H° – 140.95
2-Methyl-2-nitropropane (3×C-(H) ₃ (C))+(1×C-(C) ₃ (NO ₂))+ (3×-CH ₃ corr (quaternary))	C ₄ H ₉ NO ₂	Liquid phase $\Delta_t H^{\circ} = -216.90 -213.60 -3.30$
Literature - Calculated = Residual	Reference	1,2-Dinitroethane $(2 \times C - (H)_2(C)(NO_2)) + (1 \times NO_2 - NO_2 \text{ (corr, aliph,})$
Gas phase		Literature – Calculated = Residual
$\Delta_t H^{\circ} = -177.10 -177.11$ 0.01 Liquid phase $\Delta_t H^{\circ} = -217.20 -217.20$ 0.00	70KNO/MIR 	Gas phase $\Delta_l H^{\circ} = -101.00$ $C_{\hat{p}} = 106.28$
Solid phase $\Delta_l H^{\circ} = -229.80 -229.82$ 0.02	70KNO/MIR	Liquid phase $\Delta_l H^\circ = -165.20 - 167.00$ 1.80 $C_p^\circ = 195.48$
1,1-Dinitroethane $(1 \times C - (H)_3(C)) + (1 \times C - (H)(C)(NO_2)_2) + (1 \times -CH_3 \text{ corr (tertiary)})$	C ₂ H ₄ N ₂ O ₄	Solid phase $\Delta_t H^\circ = -178.80 -178.00 -0.80$
Literature – Calculated = Residual	Reference	1,3-Dinitropropane $(1 \times C-(H)_2(C)_2) + (2 \times C-(H)_2(C)(NO_2))$
Gas phase $\Delta_t H^\circ = -81.32$		Literature – Calculated = Residual
Liquid phase $\Delta_t H^{\circ} = -148.20 -138.59 -9.61$	68LEB/RYA2	Gas phase $\Delta_{l}H^{\circ} = -141.63$ $C_{p}^{\circ} = 129.17$
1,1-Dinitropropane $(1 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2)$	C ₃ H ₆ N ₂ O ₄ (C)(NO ₂) ₂)	Liquid phase $\Delta_t H^\circ = -215.50 -212.73 -2.77$ $C_p^\circ = 225.90$
Literature – Calculated = Residual	Keterence	
Gas phase $\Delta_t H^\circ = -100.70 -99.69 -1.01$	49HOL/DOR	1,4-Dinitrobutane $(2 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(C)(NO_2))$ Literature — Calculated = Residual
Liquid phase $\Delta_t H^\circ = -163.20 -162.14 -1.06$	68LEB/RYA2	Gas phase $\Delta_t H^\circ = -162.26$ $C_p^\circ = 152.06$

TABLE 37.	Nitro	compounds	(50)	-	Continued
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1,4-Dinitrobu (2×C-(H)	ntane (Cont 2(C)2)+(2	tinued) ×C-(H) ₂ (C)(N	IO ₂))	C ₄ H ₈ N ₂ O ₄	1,2-Dinitrobenzene (Continue) $(4 \times C_B - (H)(C_B)_2) + (2 \times C_B - (H$			$+(2\times C_B-(NO_2)(C_B)_2)+$		
	Literature	e – Calculated =	= Residual	Reference	(211102)	•	e – Calculated	= Residual	Reference	
Liquid phase $\Delta_t H^\circ = -C_p^\circ =$	-237.50	-238.46 256.32	0.96	68LEB/RYA2	Liquid phase $\Delta_t H^\circ =$	21.21	21.29	-0.08	71LEB/RYA	
Solid phase $\Delta_t H^\circ = -$	- 249.20	-256.82	7.62	68LEB/RYA2	Solid phase $\Delta_t H^\circ = C_p^\circ =$	- 1.80 186.20	1.72 186.20	-3.52 0.00	71LEB/RYA 26AND	
		× C(C)2(NO2) ernary))	2)+	C ₃ H ₆ N ₂ O ₄	1,3-Dinitrobe	enzene	(2×C _B -(NO ₂)(C₄H₄N₂O₄	
	Literatur	e – Calculated	= Residual	Reference	$(1 \times NO_2 - I)$			(CB)2) ·		
Gas phase						Literatur	e – Calculated	= Residual	Reference	
$\Delta_t H^{\circ} =$		- 122.14			Gas phase $\Delta_t H^\circ =$	53.80	63.34	- 9.54	50NIT/SEK2	
Liquid phase $\Delta_t H^\circ = -$	e - 181.20 	-181.20	0.00	68LEB/RYA2	Liquid phase					
Solid phase $\Delta_t H^\circ = C_p^\circ =$	- 192.50 206.27	-192.48 206.28	-0.02 -0.01	68LEB/RYA2 58BIL/NOL	$\Delta_t H^\circ = {}$ Solid phase $\Delta_t H^\circ = {C_p^\circ} = {}$	-6.90 -27.40 188.28	-10.46 -25.38 188.28	- 2.02 0.00	71LEB/RYA 71LEB/RYA 26AND	
Nitrobenzen (5 × C _B -(I	H)(C_B) ₂)+((1×C _B -(NO ₂)(C ₆ H ₅ NO ₂	1,4-Dinitrobe		2. G. (NO.)	(6.)	C6H4N2O	
	Literatur	re – Calculated	= Kesiduai	Reference	(4 × C _B −(H		(2×C _B -(NO ₂)(e – Calculated		Reference	
Gas phase $\Delta_t H^\circ =$	67.50	67.60	-0.10	71KUS/WAD	Gas phase					
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	e 12.50 186.70 224.30	12.50 186.70 224.30 -437.36 142.90 -57.64	0.00 0.00 0.00	71LEB/KAT2 36PAR/TOD 36PAR/TOD	$C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \Delta_{f}G^{\circ} = S^{\circ}$	-14.40	52.34 -23.96 237.32 275.38 -621.79 161.43	9.56	26AND/LYN	
	$H)(C_B)_2) + O(C_B)_2$	(2×C _B -(NO ₂)(corr)) re – Calculated		C₄H₄N₂O₄ Reference	$C_{\rho}^{\circ} = S^{\circ} =$	-38.70 192.00	- 65.12 - 38.88 182.44 311.92	0.18 9.56	71LEB/RYA 26AND/LYN	
Gas phase Δ _i H° =		96.34			$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f = -$		- 585.25 135.61 - 54.70			

TABLE	37.	Nitro	compounds	(50)	_	Continued

T.	ABLE 37. N	itro compound	ls (50) — Co	ontinued	TABLE 37. Nitro compounds (50) — Continued				
		3×C _B -(NO ₂)(0 corr))	C _B)₂)+	C ₆ H ₃ N ₃ O ₆	$(1 \times C - (H))$)3(C))+(4×		ene 2)+(1×C _B -(C) H ₃ (ortho corr)	
	Literature	e – Calculated =	= Residual	Reference	Literature - Calculated = Residual Reference				Reference
Gas phase Δ _i H° =	70.10	70.08	0.02	78CUN/PAL	Solid phase $\Delta_t H^\circ =$		-35.22		
Liquid phase $\Delta_t H^\circ =$	- 20.50	-19.92	-0.58	71LEB/RYA	(1×C-(H) ₃ (C))+(4×		ene 2) + (1 × C _B -(C) H ₃ (meta corr)	
Solid phase $\Delta_f H^\circ = C_p^\circ =$	-37.20	-37.41 230.79	0.21	71LEB/RYA		Literat	ure – Calcula	ted = Residual	Reference
			$(C_B)_2) + (1 \times C_B)_2$	$C_{10}H_7NO_2$ C_{B} - $(NO_2)(C_B)_2) +$	Liquid phase Δ _t H° =	-31.50	-28.11	-3.39	71LEN/VEL
		e – Calculated =	= Residual	Reference	-) ₃ (C))+(4×	e; 4-Nitrotolu (C _B –(H)(C _B);	ene $(1 \times C_B - (C))$	$C_7H_7NO_2$ $(C_B)_2) +$
Gas phase $\Delta_t H^\circ =$	149.70	135.42	14.28	50NIT/SEK2		Literature	- Calculated	= Residual	Reference
Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f =$	e	60.48 251.10 270.96 -544.23 222.74 -89.85			Gas phase $\Delta_{l}H^{\circ} = {}$ Liquid phase $\Delta_{l}H^{\circ} = {}$ $C_{p}^{\circ} = $ $S^{\circ} = {}$	31.00	- 24.11 210.60 259.23	-4.17	70LEN/VEL
Solid phase $\Delta_t H^\circ =$	42.60	41.41	1.19	37BAD	$\Delta_{r}S^{\circ} = \Delta_{f}G^{\circ} = InK_{f} = InK_{f}$		538.74 136.52 55.07		
$C_p^{\circ} - S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f =$		196.47 257.71 -557.48 207.62 -83.75			Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	-48.12 172.38	-39.22 175.67 252.65 -545.32	-8.90 -3.29	71LEN/VEL 79RIC/SAV
(1×C-(H	I) ₃ (C))+(4 NO ₂)(C _B) ₂)	ie; 2-Nitrotolue $\times C_B$ -(H)(C _B) ₂ + (1 × NO ₂ -CH	$+ (1 \times C_{B} - (C_{B}) + (1 \times C_{B})$))	$\Delta_t G^\circ = InK_t = InK_t$ Nitromethylk		123.37 - 49.77 enylnitrometh		C₁H₁NO₂
	Literatur	e – Calculated :	- Mesiduai	Reference	(3 × CB-(F		- Calculated	s) ₂) + (1 × C–(H = Residual	Reference
Gas phase $\Delta_i H^\circ =$		37.17			Gas phase				

Gas phase $\Delta_t H^\circ =$

Liquid phase $\Delta_t H^\circ = -22.80$

30.70

30.69

-22.80

0.01

0.00

69PEP/LEB

69PEP/LEB

Liquid phase $\Delta_t H^\circ =$

- 9.70

- 22.11

12.41

71LEN/VEL

TABLE 3	7 Nitro	compounds	(50)	_	Continued

	Literature - Calculated = Residual	Reference	$(3 \times C_B-(NO_2)(C_B)_2) + (3 \times NO_2-NO_2 \text{ (meta corr)}) + (2 \times NO_2-CH_3 \text{ (ortho corr)})$
			Literature – Calculated = Residual Reference
Solid phase $\Delta_t H^\circ =$	- 34.45	<u> </u>	Liquid phase $\Delta_t H^\circ = -52.53$
$(2 \times C_{B} - ($	toluene H) ₃ (C)) + $(3 \times C_B - (H)(C_B)_2) + (1 \times C_B - (C) + (1 \times NO_2)(C_B)_2) + (1 \times NO_2 - CH_3 (ortho corr))$ -NO ₂ (meta corr))		Solid phase $\Delta_t H^{\circ} = -66.90 - 68.78$ 1.88 39BUR/THO
	Literature – Calculated = Residual	Reference	2-Nitrophenol; o-Nitrophenol C_6H_5NO $(4 \times C_B-(H)(C_B)_2) + (1 \times C_B-(O)(C_B)_2) + (1 \times C_B-(NO_2)(C_B)_2) + (1 \times O-(H)(C_B)) + (1 \times NO_2-OH (ortho corr))$
Gas phase $\Delta_t H^\circ =$	30.00 32.91 -2.91	77PEL	Literature - Calculated = Residual Reference
Liquid pha Δ _ι H° =	se - 45.07		Gas phase $\Delta_i H^{\circ} = -129.00 -101.26 -27.74$ 92RIB/REI
Solid phase Δ _t H° =	-65.80 -60.75 -5.05	43PRO/GIL	Liquid phase $\Delta_t H^\circ = -177.02$
	toluene $H_{3}(C) + (3 \times C_{B}-(H)(C_{B})_{2}) + (1 \times C_{B}-(C)(C_{B})_{2}) + (2 \times NO_{2}-CH_{3} \text{ (ontho corr)})$		Solid phase $\Delta_t H^{\circ} = -202.40 - 191.63 - 10.77$ 92RIB/REI
(1×NO ₂	-NO ₂ (meta corr)) Literature - Calculated = Residual		4.27
	Enterature - Calculated = Residual	Reference	3-Nitrophenol; m-Nitrophenol $(4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (O)(C_B)_2) + (1 \times C_B - (NO_2)(C_B)_2) + (1 \times O - (H)(C_B)) + (1 \times NO_2 - OH (meta corr))$
Gas phase Δ _t H° =	51.90 34.91 16.99	Reference 77PEL	$(4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (O)(C_B)_2) + (1 \times C_B - (NO_2)(C_B)_2) +$
$\Delta_t H^{\circ} =$	51.90 34.91 16.99		$(4 \times C_B-(H)(C_B)_2) + (1 \times C_B-(O)(C_B)_2) + (1 \times C_B-(NO_2)(C_B)_2) + (1 \times O-(H)(C_B)) + (1 \times NO_2-OH (meta corr))$
Liquid pha	51.90 34.91 16.99 se -43.07		$(4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (O)(C_B)_2) + (1 \times C_B - (NO_2)(C_B)_2) + (1 \times O - (H)(C_B)) + (1 \times NO_2 - OH \ (meta \ corr))$ $Literature - Calculated = Residual \qquad Reference$ Gas phase
$\Delta_t H^{\circ} =$ Liquid pha $\Delta_t H^{\circ} =$ Solid phase $\Delta_t H^{\circ} =$ 2,4,6-Trinit $(1 \times C - (I \times C_{B^{-1}}))$	51.90 34.91 16.99 se -43.07 -46.40 -56.75 10.35	77PEL 49MED/THO C ₇ H ₅ N ₃ O ₆ (C _B) ₂) +	$(4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (O)(C_B)_2) + (1 \times C_B - (NO_2)(C_B)_2) + (1 \times O - (H)(C_B)) + (1 \times NO_2 - OH \ (meta \ corr))$ Literature – Calculated = Residual Reference Gas phase $\Delta_t H^\circ = -105.50 - 105.26 - 0.24 92RIB/REI$ Solid phase $\Delta_t H^\circ = -205.70 - 204.63 - 1.07 92RIB/REI$
$\Delta_t H^{\circ} =$ Liquid pha $\Delta_t H^{\circ} =$ Solid phase $\Delta_t H^{\circ} =$ 2,4,6-Trinit $(1 \times C - (I \times C_{B^{-1}}))$	51.90 34.91 16.99 se -43.07 -46.40 -56.75 10.35 rotoluene H ₃ (C)) + (2 × C _B -(H)(C _B) ₂) + (1 × C _B -(C)(NO ₂)(C _B) ₂) + (3 × NO ₂ -NO ₂ (meta corr))	77PEL 49MED/THO C ₇ H ₅ N ₃ O ₆ (C _B) ₂) +	$(4 \times C_B-(H)(C_B)_2) + (1 \times C_B-(O)(C_B)_2) + (1 \times C_B-(NO_2)(C_B)_2) + (1 \times O-(H)(C_B)) + (1 \times NO_2-OH \ (meta \ corr))$ $Literature - Calculated = Residual \qquad Reference$ $Gas \ phase \\ \Delta_t H^\circ = -105.50 \qquad -105.26 \qquad -0.24 \qquad 92RIB/REI$ $Solid \ phase \\ \Delta_t H^\circ = -205.70 \qquad -204.63 \qquad -1.07 \qquad 92RIB/REI$ $4-Nitrophenol; \ p-Nitrophenol \qquad C_4H_5NO_3 \\ (4 \times C_B-(H)(C_B)_2) + (1 \times C_B-(O)(C_B)_2) + (1 \times C_B-(NO_2)(C_B)_2) + (1 \times O-(H)(C_B))$

TABLE	27	Nitro	compounds	(50)	_	Continued
LABLE	.) /.	NILLO	compounds	LOUL	_	Continued

4-Nitrophenol; p-N $(4 \times C_B-(H)(C_B);$ $(1 \times O-(H)(C_B))$	$(1 \times C_B - (O))(C_E)$		$C_6H_5NO_3$ (NO_2)(C_B) ₂) +	2,4,6-Trinit $(2 \times C_{B} - (1 \times O - (1 \times O - (1 \times O \times $
Liter	ature - Calculated	= Residual	Reference	
I iquid abose				
Liquid phase $\Delta_t H^\circ =$	- 193.02			Gae phaca
	- 193.02 248.37			Gas phase
$C_p^{\circ} =$				$\Delta_{\rm f}H^{\circ} =$
S° =	228.73			
$\Delta_f S^\circ =$	-535.45			
$\Delta_t G^\circ =$	-33.37			Liquid pha
$lnK_f =$	13.46			$\Delta_{\mathbf{f}}H^{\circ} =$
Solid phase				Solid phase
$\Delta_t H^\circ = -212.4$	10 - 204.63	-7.77	92RIB/REI	$\Delta_{\rm f}H^{\circ} =$
$C_p^{\circ} =$	160.44		/21X1D/1X151	- H
S° =	231.67			
Δ ₆ S° =	-532.51			
$\Delta_{i}G^{\circ} =$	-352.51 -45.86			2 Nitroanil
$\ln K_t =$	18.50			2-Nitroanil
ink _t =	18.50			(4×С _в ((1×N(1
	$(2) + (2 \times C_B - (NO_2))$ $(2) + (1 \times NO_2 - NO_2)$ (2) + (2) + (2) + (2) (3) + (2) + (2) (4) +		.в-(О)(Св <i>)2)</i> т	Gas phase $\Delta_t H^\circ =$
Lite	rature – Calculated	= Residual	Reference	Liquid pha
Gas phase $\Delta_t H^\circ = -128.1$	10 -105.52	- 22.58	58HOY/PEP	$\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} =$
Liquid phase Δ _f H° =	- 199.98			$\Delta_{f}G^{\circ} = \ln K_{t} -$
Solid phase $\Delta_t H^\circ = -235.6$	80 -217.16	-18.64	42BAD	Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$
) ₂) + (2 × C _B -(NO ₂)) + (1 × NO ₂ -NO ₂ (ortho corr))		C ₆ H ₄ N ₂ O ₄ C _B -(O)(C _B) ₂) +	$\Delta_f S^\circ = \\ \Delta_f G^\circ = \\ \ln K_f = $
	rature – Calculated	= Residual	Reference	3-Nitroanili (4×C _B -(
	··· <u>·</u>			$(1 \times C_{B}-($
Gas phase $\Delta_t H^\circ = -97.5$	80 -95.52	-2.28	58HOY/PEP	
Liquid phase $\Delta_t H^\circ =$	- 183.98			Gas phase $\Delta_l H^\circ =$

Solid phase $\Delta_t H^\circ = -209.90$

-204.16

-5.74

42BAD

	Literatur	e – Calculated	= Residual	Reference
Gas phase				
$\Delta_f H^\circ =$		- 88.78		· · · · · · · · · · · · · · · · · · ·
Liquid phas	se			
$\Delta_t H^\circ =$		- 193.44		
Solid phase	;			
$\Delta_{\rm f}H^{\circ} =$	-213.97	-216.19	2.22	60VOR/PRI
2-Nitroanili		$(1 \times C_{B} - (NO_{2}))$	(C).)±(1×C	C ₆ H ₆ N ₂
		$1 \times NH_2-NO_2$		B-(14)(CB)2)+
(1 > 14-(1	1)2(CB)) T (
(1 ^ 1 ^ (1	, , ,, ,	e – Calculated		Reference
	, , ,, ,			Reference
	, , ,, ,			
Gas phase $\Delta_t H^\circ =$	Literatur 63.80	re – Calculated	= Residual	Reference 58HOY/PEF
Gas phase $\Delta_t H^\circ =$ Liquid phas	Literatur 63.80	e – Calculated	= Residual	58НОУ/РЕР
Gas phase $\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$	Literatur 63.80	re – Calculated	= Residual	
Gas phase $\Delta_t H^\circ =$ Liquid phas $\Delta_t H^\circ =$ $C_\rho^\circ =$	Literatur 63.80	67.74 -9.16	= Residual	58НОУ/РЕР
Gas phase $\Delta_t H^\circ =$ Liquid phas $\Delta_t H^\circ =$	Literatur 63.80	67.74 - 9.16 241.63	= Residual	58НОУ/РЕР
Gas phase $\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$	Literatur 63.80	67.74 - 9.16 241.63 242.71	= Residual	58НОУ/РЕР
Gas phase $\Delta_t H^\circ =$ Liquid phas $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$	Literatur 63.80	67.74 - 9.16 241.63 242.71 - 579.99	= Residual	58НОУ/РЕР
Gas phase $\Delta_t H^\circ =$ Liquid phas $\Delta_t H^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	63.80 se -9.40	67.74 - 9.16 241.63 242.71 - 579.99 163.76	= Residual	58НОУ/РЕР
Gas phase $\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t -$ Solid phase $\Delta_t H^\circ =$	63.80 se -9.40	67.74 - 9.16 241.63 242.71 - 579.99 163.76	= Residual	58НОУ/РЕР
Gas phase $\Delta_t H^\circ =$ Liquid phas $\Delta_t H^\circ =$ $C_t^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$ Solid phase	63.80 se -9.40	-9.16 241.63 242.71 -579.99 163.76 -66.06	= Residual - 3.94 - 0.24	58HOY/PEF 71LEB/GUT
Gas phase $\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t -$ Solid phase $\Delta_t H^\circ =$	63.80 se -9.40	-9.16 241.63 242.71 -579.99 163.76 -66.06	- 3.94 - 0.24	58HOY/PEP 71LEB/GUT 71LEB/GUT
Gas phase $\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\ln K_t =$ Solid phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $S^\circ =$	63.80 se -9.40	-9.16 241.63 242.71 -579.99 163.76 -66.06	- 3.94 - 0.24	58HOY/PEP 71LEB/GUT 71LEB/GUT
Gas phase $\Delta_t H^\circ =$ Liquid phase $C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t -$ Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	63.80 se -9.40	- 9.16 241.63 242.71 - 579.99 163.76 - 66.06	- 3.94 - 0.24	58HOY/PEP 71LEB/GUT 71LEB/GUT

Literature - Calculated = Residual

61.74

-3.34

58.40

Reference

73MAL/GIG2

TABLE 37. Nitro compounds (50) - Continued

	$H)(C_B)_2) + ($	ed) 1×C _B -(NO ₂)(1×NH ₂ -NO ₂		$C_6H_6N_2O_2$ $I-(H)_2(C_B)) +$	2. 2,3-Dinitroaniline (Continued) $C_6H_5N_3$ $(3 \times C_B-(H)(C_B)_2) + (2 \times C_B-(NO_2)(C_B)_2) + (1 \times N-(H)_2(C_B)) +$ $(1 \times C_B-(N)(C_B)_2) + (1 \times NO_2-NO_2 \ (ortho \ corr)) +$ $(1 \times NH_2-NO_2 \ (ortho \ corr)) + (1 \times NH_2-NO_2 \ (meta \ corr))$				
	Literature	e – Calculated	= Residual	Reference	•	rature – Calculated	,	Reference	
Liquid phas									
$\Delta_t H^\circ = C_p^\circ = S^\circ =$	– 14.40	- 15.16 241.63 242.71	0.76	71LEB/GUT	Liquid phase $\Delta_t H^\circ =$	-10.37			
Δ _t S° =		- 579.99							
$\Delta_f G^\circ = \ln K_f =$		157.76 - 63.64			Solid phase $\Delta_t H^\circ = -11.7$ $C_p^\circ =$	0 -30.66 205.07	18.96	62ZAK/ALE	
Solid phase									
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	-38.30 168.20	-28.23 170.48 233.89 -588.81 147.32	-10.07 -2.28	71LEB/GUT 26AND/LYN				$C_6H_5N_3O_6$ $I-(H)_2(C_B)) +$ $NO_2 (meta corr)) +$	
lnK _f	-59.43				Liter	ature – Calculated	= Residual	Reference	
4-Nitroanili (4×C _B -((1×N-(F	H)(C _B) ₂)+((1 × C ₂₂ –(NO ₂)	(C _B) ₂) + (1 × C	$C_6H_6N_2O_2$ $C_B=(N)(C_B)_2) +$	Gas phase Δ _t H° =	81.76			
	Literatur	e – Calculated	= Residual	Reference	Liquid phase $\Delta_t H^\circ =$	-13.42			
Gas phase $\Delta_t H^\circ =$	58.80	71.74	-12.94	73MAL/GIG2	Solid phase $\Delta_t H^\circ = -65.66$	0 –26.19	- 39.41	62ZAK/ALE	
Liquid phas					 				
$\Delta_t H^\circ = C_r^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	-20.70	-5.16 241.63 242.71 -579.99 167.76	- 15.54	71LEB/GUT		$(2) + (2 \times C_B - (NO_2))$ + (1 \times NH_2 - NO_2)			
$lnK_f =$		-67.67				ature – Calculated	= Residual	Reference	
Solid phase									
$\Delta_{\ell}H^{\circ} = C_{p}^{\circ} = S^{\circ} = A^{\circ}S^{\circ} = A^{\circ}S^{\circ$	-42.90 169.03	- 18.23 170.48 233.89	-24.67 -1.45	71LEB/GUT 26AND/LYN	Gas phase Δ _t H° =	42.48	·		
$\Delta_f S^\circ = \Delta_f G^\circ =$		-588.81 157.32			Liquid phase				
$\ln K_{\rm f} =$	-63.46	20,102			$\Delta_{\rm f}H^{\circ} =$	-55.62			
					$C_p^{\circ} =$	292.25			
					S° = Δ _ι S° =	293.79 764.41			
2,3-Dinitro	niline			C ₆ H ₅ N ₃ O ₄	$\Delta_i G^\circ =$	172.29			
$(3 \times C_B - (1 \times C_B $	$H)(C_B)_2) + (N)(C_B)_2) + (N)(C_B)_2$	$(2 \times C_B - (NO_2))$ $(1 \times NO_2 - NO_2)$ $(1 \times NO_2 + (1 \times NO_2))$	(ortho corr))-	I−(H) ₂ (C _B)) + +	$lnK_f =$	-69.50			
(1 × INF12*	-14C) (OLNO	. ani))+(1 X [M12™NU2 (ME	ш сантуу	Solid phase				
	Literatur	e – Calculated	= Residual	Reference	$\Delta_t H^\circ = -44.30$ $C_p^\circ =$	0 - 71.26 201.31	26.96	62ZAK/ALE	
					$S^{\circ} =$	321.60			
					$\Delta_{f}S^{\circ} =$	-731.60			
(tas phace					$\Delta_t G^{\circ} =$	148.36			
Gas phase $\Delta_t H^\circ =$		86.48			$\ln K_{\rm f} = -59.85$				

TABLE 37. Nitro compounds (50) — Continue	TABLE 37	. Nitro	compounds	(50)) —	Continue
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2,6-Dinitroaniline $C_6H_5N_3O_4$ $(3 \times C_B-(H)(C_B)_2) + (2 \times C_B-(NO_2)(C_B)_2) + (1 \times C_B-(N)(C_B)_2) + (1 \times N-(H)_2(C_B)) + (1 \times NO_2-NO_2 \ (\textit{meta} \ \textit{corr})) + (2 \times NH_2-NO_2 \ (\textit{ortho} \ \textit{corr}))$	2,4,6-Trinitroaniline; Picramide $C_4H_4N_4C_2 + C_8-(H)(C_B)_2 + (1 \times C_B-(N)(C_B)_2) + (3 \times C_B-(NO_2)(C_B)_2) + (1 \times N-(H)_2(C_B)) + (3 \times NO_2-NO_2 \ (meta \ corr)) + (2 \times NH_2-NO_2 \ (ortho \ corr))$					
Literature - Calculated = Residual Reference	Literature – Calculated = Residual Reference					
Gas phase $\Delta_i H^\circ = 59.48$	Gas phase $\Delta_t H^\circ = 41.70$ 66.22 -24.52 78CUN/PAL					
Liquid phase $\Delta_t H^{\circ} = -36.12$	Liquid phase $\Delta_t H^\circ = -45.58$					
Solid phase $\Delta_t H^\circ = -50.60 -51.76$ 1.16 62ZAK/ALE $C_\rho^\circ = 207.15$	Solid phase $\Delta_t H^\circ = -83.60 -63.79 -19.81$ 49MED/TOM $C_p^\circ = 249.66$					
$ \begin{array}{ll} \textbf{3,4-Dinitroaniline} & C_6H_5N_3O_4\\ (3\times C_{B^-}(H)(C_B)_2) + (2\times C_{B^-}(NO_2)(C_B)_2) + (1\times N-(H)_2(C_B)) + \\ (1\times C_{B^-}(N)(C_B)_2) + (1\times NH_2-NO_2\ (\textit{meta}\ corr)) + \\ (1\times NO_2-NO_2\ (\textit{meta}\ corr)) \end{array} $	$ \begin{array}{ll} \textbf{2-Nitrobenzoic acid} & \textbf{C}_7\textbf{H}_5\textbf{NO}_4\\ (4\times\textbf{C}_B-(\textbf{H})(\textbf{C}_B)_2) + (1\times\textbf{C}_B-(\textbf{NO}_2)(\textbf{C}_B)_2) + (1\times\textbf{C}_B-(\textbf{CO})(\textbf{C}_B)_2) + \\ (1\times\textbf{CO}-(\textbf{O})(\textbf{C}_B)) + (1\times\textbf{O}-(\textbf{H})(\textbf{CO})) + (1\times\textbf{NO}_2-\textbf{COOH}\\ (\textit{ortho}~\textit{corr})) \end{array} $					
Literature - Calculated = Residual Reference	Literature - Calculated = Residual Reference					
Gas Phas $\Delta_t H^{\circ} = 57.48$	Gas phase $\Delta_l H^\circ = -285.01$					
Liquid phase $\Delta_t H^\circ = -38.12$	Liquid phase $\Delta_t H^\circ = -378.80 - 380.80$ 2.00 71LEB/RYA $C_\rho^\circ = 254.39$					
Solid phase $\Delta_t H^\circ = -32.60 -53.76$ 21.16 62ZAK/ALE $C_p^\circ = 207.15$	Solid phase $\Delta_t H^\circ = -398.48 -400.38$ 1.90 71LEB/RYA $C_\rho^\circ = 191.63$ 176.94 14.69 26AND/LYN $S^\circ = 255.45$					
3,5-Dinitroaniline $C_6H_5N_3O_4$ $(3 \times C_B-(H)(C_B)_2) + (2 \times C_B-(NO_2)(C_B)_2) + (1 \times C_B-(N)(C_B)_2) + (1 \times N-(H)_2(C_B)) + (1 \times NO_2-NO_2 \ (meta\ corr)) + (2 \times NH_2-NO_2 \ (meta\ corr))$	$\Delta_{\ell}S^{\circ} = -616.99$ $\Delta_{\ell}G^{\circ} = -216.42$ $\ln K_{\ell} = 87.30$					
Literature - Calculated = Residual Reference	3-Nitrobenzoic acid $C_6H_5NO_4$ $(4 \times C_B-(H)(C_B)_2) + (1 \times C_B-(NO_2)(C_B)_2) + (1 \times C_B-(CO)(C_B)_2) + (1 \times CO-(O)(C_B)) + (1 \times O-(H)(CO)) + (1 \times NO_2-COOH$					
Gas phase $\Delta_t H^\circ = 47.48$	(meta corr)) Literature – Calculated = Residual Reference					
Liquid phase $\Delta_t H^\circ = -48.12$	Gas phase $\Delta_t H^{\circ} = -296.01$					
Solid phase $\Delta_t H^\circ = -38.90 -63.76$ 24.86 62ZAK/ALE $C_p^\circ -$ 207.15	Liquid phase $\Delta_t H^\circ = -394.70 -394.80 0.10$ 71LEB/RYA $C_p^\circ = 254.39$					

TABLE 37. Nitro compounds (50) - Continued

TABLE 38. Nitrites (3)

	$H)(C_B)_2) +$			$C_6H_5NO_4$ $C_B-(CO)(C_B)_2) +$	Methyl nitr (1×C-(I		×O-(C)(NO)), $\sigma = 3$	CH₃ONO
	-COOH (m		,,			Literatui	re – Calculated	= Residual	Reference
	Literatu	re – Calculated	= Residual	Reference					
					Gas phase	CE 40	66.40	1.00	(0D 411/0DD
					$\Delta_f H^\circ =$	-65.40	-66.49	1.09	62RAY/GER
Solid phase		444.20	0.62	711 ED/D3/4	$C_p^{\circ} =$	63.22	63.22	0.00	69STU/WES
	-414.01	-411.38	-2.63	71LEB/RYA	S° =	284.30	284.30	0.00	69STU/WES
$C_p^{\circ} =$	173.22	176.94	-3.72	26AND/LYN	$\Delta_f S^\circ =$		- 115.57		
s° =		255.45			$\Delta_{\rm f}G^{\circ} =$		- 32.03		
$\Delta_f S^\circ =$		-611.25			$lnK_f =$		12.92		
$\Delta_{\mathbf{f}}G^{\circ} =$		-229.13							
$lnK_f =$		92.43							
		······························		- Paragraphic -	Ethyl nitrit (1×C-(F		× C-(H) ₂ (O)(0	C))+(1×O-(0	C₂H₅ONO
	$H)(C_B)_2) +$	(1×C _B -(NO ₂)((1×O-(H)(CO		$C_7H_5NO_4$ $C_8-(CO)(C_B)_2) +$		Literatur	e – Calculated	= Residual	Reference
Gas phase	Literatu	re – Calculated	= Residual	Reference	Gas phase $\Delta_t H^a = C_p^a =$	- 101.25	- 99.39 83.55	-1.86	56GRA
$\Delta_t H^\circ =$		-310.01			Liquid phas	se			
					$\Delta_i H^\circ =$	-127.60	- 129.91	2.31	59GRA/WIL
iquid phas									
$\Delta_{\mathbf{f}}H^{\circ} = C_{p}^{\circ} =$	- 392.20	-410.80 254.39	18.60	71LEB/RYA					
Solid phase Δ _e H° =	-426.90	-425.38	1.52	71LEB/RYA	<i>n-</i> Propyl ni (1×C-(F (1×O-(C	H)3(C))+(1	\times C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂ (C₃H₇ONO O)(C)) +
-		176.94	3.39			T itomotum	o Coloulated	Donishuni	D = 6
$C_p^{\circ} = S^{\circ} =$	180.33	255.45	3.39	26AND/LYN		Literatur	e – Calculated	= Kesiduai	Reference
-									
$\Delta_{\rm f}S^{\circ} =$		-616.99			.				
$\Lambda_i G^{\circ} =$		- 241.42 07.20			Gas phase	105.04	100.00	5.00	50.00 t #15-
$lnK_f =$		97.39	······································		$\Delta_t H^\circ = C_p^\circ =$	- 125.94	-120.02 106.44	-5.92	59GRA/WIL

Table 39. Nitrates (6)

<u> </u>		TABLE 39. Ni	trates (6)			TABLE	39. Nitrates (6) – Continu	ued
Methyl nit (1×C-(× O-(C)(NO ₂)), σ = 6	CH ₃ ONO ₂	(1×C-(1	itrate (Cont H) ₃ (C)) + (1 C)(NO ₂)), o	\times C-(H) ₂ (C) ₂)	+ (1×C-(H) ₂	C ₃ H ₇ ONO ₂ (O)(C)) +
·	Literatu	re – Calculated	= Residual	Reference	((//-	re – Calculated	= Residual	Reference
Gas phase	.								
$\Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$	-123.00 76.48 301.88	-121.97 77.19 304.34 -198.05 -62.92 25.38	- 1.03 - 0.71 - 2.46	58RAY/OGG2 69STU/WES 69STU/WES	Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	se -214.51	-218.10 196.94 275.77 -499.24 -69.25 27.94	3.59	57FAI/SKI
Liquid ph	ase								
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	-157.10 157.19 216.98	- 156.57 132.88 210.80 - 291.59 - 69.63 28.09	-0.53 24.31 6.18	58RAY/OGG2 53GRA/SMI 53GRA/SMI		H) ₃ (C))+(1 C)(NO ₂))+	×C-(H)(O)(C (2×-CH ₃ corr re – Calculated	(tertiary)), σ	
Ethyl nitr (1×C-		×C-(H)2(O)(0	C))+(1×O-(0	$C_2H_5ONO_2$ C)(NO ₂)), $\sigma = 6$	Gas phase $ \Delta_i H^\circ = C_p^\circ = S^\circ = $	-191.00 120.67 373.21	-188.21 120.70 369.73	-2.79 -0.03 3.48	57GRA/PRA 69STU/WES 69STU/WES
	Literatu	re – Calculated	= Residual	Reference	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	0,0181	-405.28 -67.37 27.18		0,010,1120
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 154.10 97.36 348.32	-154.87 97.52 347.77 -290.93 -68.13 27.48	0.77 - 0.16 0.55	57GRA/PRA 69STU/WES 69STU/WES	Liquid pha $ \Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ $	se 229.70 191.10 263.20	- 229.54 194.92 268.79 - 506.22 - 78.61 31.71	- 0.16 - 3.82 - 5.59	57FAI/SKI 88LUS/RUB 88LUS/RUB
Liquid ph					$lnK_f =$		31./1		
$\Delta_t H^\circ = C_r^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	- 190.41 170.30 247.20	-192.37 166.52 243.39 -395.31 -74.51	1.96 3.78 3.81	57FAI/SKI 54GRA/SMI 54GRA/SMI	(2×C-(1		te; EGDN + (2×O-(C)(N 2) (aliphatic co		C ₂ H ₄ N ₂ O ₆
$lnK_t =$		30.06				Literatuı	re – Calculated	= Residual	Reference
		$1 \times C - (H)_2(C)_2$ $\sigma = 6$	+(1×C-(H) ₂	C ₃ H ₇ ONO ₂ (O)(C))+	Gas phase $\Delta_t H^\circ =$	-189.30	195.02	5.72	77PEL
	Literatu	re – Calculated	= Residual	Reference	Liquid pha Δ _I H° =	se 255.80	-257.72	1.92	34TOM/TAK
Gas phas $\Delta_t H^\circ - C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ - \ln K_f =$	e - 173.89 121.29 385.35	- 175.50 120.41 386.93 - 388.08 - 59.79 24.12	1.61 0.88 -1.58	57GRA/PRA 69STU/WES 69STU/WES					

TABLE 39. Nitrates (6) - Continued

TABLE 40. Nitramines (10)

	TABLE	39. Nitrates (6) – Continu	ed	Table 40. Nitramines (10)				
(1 × C-(H) ₂ (O)(C)) -)(O)(C) ₂ (roglycerine + (3 × O-(C)(N ethers,esters)) 2) (aliphatic co	+	C ₃ H ₅ N ₃ O ₉	Nitrourea (1×N-(H) (1×N-(H)		mides, ureas))+	(1×CO-(N) ₂)	CH₃N₃O₃ +
(3×(ONC		e – Calculated		Reference		Literat	ure-Calculated =	= Residual	Reference
Gas phase $\Delta_l H^\circ =$		-279.09	-0.61	88MIR/KOR	Solid phase $\Delta_t H^\circ = -$	- 282.30	-282.35	0.05	49MED/THO
Liquid phas $\Delta_t H^\circ =$		- 371.78	0.08	88MIR/KOR	Methyldinitro (1×C-(H) (1×N-(C)	(3(N)) + (1	×-CH₃ corr (q	uaternary))+	CH₃N₃O₄
						Literatu	re – Calculated =	= Residual	Reference
					Gas phase $\Delta_t H^\circ =$	53.50	53.48	0.02	87MIR/KOR
					Liquid phase Δ _f H° =	1.50	1.50	0.00	87MIR/KOR
					Methylenedia (1×C-(H)		MEDINA 2×N-(H)(C)(N	O ₂))	CH ₄ N ₄ O ₄
						Literat	ure-Calculated =	= Residual	Reference
					Solid phase $\Delta_t H^\circ =$	- 57.90	- 59.00	1.10	54MUR/GOL
					Dimethylnitr (2×C-(H) (1×N-(C)	$_{3}(N)) + (2$	×-CH₃ corr (qı	uaternary))+	C ₂ H ₆ N ₂ O ₂
						Literatu	re – Calculated =	Residual	Reference
					Gas phase $\Delta_t H^\circ =$	-5.00	- 5.64	0.64	71MAT/V'Y
					Liquid phase $\Delta_t H^\circ =$,	- 54.00	1 - Table 1 - 2 - Table 1 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 -	
					Solid phase $\Delta_t H^\circ =$	- 74.90	- 62.18	- 12.72	71MAT/V'Y
					Ethylenedini (2×C-(H)		Haleite + (2×N-(H)(C)	(NO ₂))	C₂H₄N₄O₄
						Literat	ure-Calculated =	Residual	Reference
					Solid phase $\Delta_t H^\circ = -C_p^\circ =$	- 104.60	- 101.00 175.30	-3.60	73KRI/LIC

TARIF 4	40.	Nitrramines	(10)	_	Continued

TABLE 40.	Nitramines (10)	 Continued

Diethylnitr (2×C-())+(1×N-(C	$C_4H_{10}N_2O$ $C)_2(NO_2))$		
***************************************	Reference			
Gas phase $\Delta_t H^\circ =$	-53.10	-53.12	0.02	58CAS/FLE
Liquid pha $\Delta_t H^\circ =$	ase 106.20	-106.82	0.62	58CAS/FLE

N-Nitropiperidine $C_5II_{10}N_2O_2$ $(3 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(C)(N)) + (1 \times N - (C)_2(NO_2)) +$ (1×N-Nitropiperidine rsc)

Literatur	Reference		
Gas phase $\Delta_t H^\circ = -44.40$	- 44.40	0.00	71MAT/V'Y
Liquid phase $\Delta_f H^\circ = -92.90$	- 92.90	0.00	71MAT/V'Y
Solid phase $\Delta_t H^{\circ} = -107.75$	- 107.75	0.00	87MES/TOD

1,3,5-Cyclotrimethylenetrinitramine;

Hexogen; RDX

 $C_3H_6N_6O_6$ $(3 \times C - (H)_2(N)_2) + (3 \times N - (C)_2(NO_2)) + (1 \times RDX \text{ rsc})$

	Literature	- Calculated	Reference		
Gas phase $\Delta_t H^\circ =$	205.30	206.00	-0.70	78CUN/PAL	
Solid phase $\Delta_t H^\circ =$	71.00	72.00	-1.00	73KRI/LIC	

1,3,5,7-Cyclotetramethy	lenetetranitramine;
Octogen: HMY	

C₄H₈N₈O₈

 $(4 \times C - (H)_2(N)_2) + (4 \times N - (C)_2(NO_2)) + (1 \times HMX \text{ rsc})$

	Literature	e – Calculated	alated = Residual Reference			
Gas phase $\Delta_t H^\circ =$	248.90	249.00	-0.10	78CUN/PAL		
Solid phase $\Delta_t H^\circ =$	87.90	88.00	-0.10	73KRI/LIC		

N-Methyl-N-nitro-(2,4,6-trinitro)aniline; Tetryl;

Tetralite

C7H5N5O8

 $(2 \times C_{B}-(H)(C_{B})_{2}) + (1 \times C_{B}-(N)(C_{B})_{2}) + (3 \times C_{B}-(NO_{2})(C_{B})_{2}) + (1 \times N-(C)(C_{B})(NO_{2})) + (1 \times C-(H)_{3}(N))$

	Literature	- Calculated	Reference		
Gas phase $\Delta_t H^\circ =$	162.80	162.71	0.09	78CUN/PAL	
Liquid phas $\Delta_t H^\circ =$	se 52.00	52.31	-0.31	73KRI/LIC	
Solid phase $\Delta_f H^\circ =$	29.00	29.07	- 0.07	73KRI/LIC	

TABLE 41. Cyclic CHNO (3)

TABLE 42	2. Thiols	(31)
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Succinimide $(2 \times C - (H)_2(CO)(C)) + (2 \times (1 \times \text{succinimide rsc})$	×CO-(C)(N))+(1	$C_4H_5NO_2$ 1 × N-(H)(CO) ₂)+	Methanethi (1×C–(F		×S-(C)(H)),	r = 3	CH ₄ !
Literature — C	Calculated = Residu	al Reference		Literatu	re – Calculated	l = Residual	Reference
	375.50 0.0	0 90MEN/PIL	Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = 0$	- 22.97 50.25 255.06	-23.62 51.49 255.86 -43.08	0.65 - 1.24 - 0.80	61GOO/LAC 69STU/WES 69STU/WES
Solid phase $\Delta_t H^\circ = -459.10 -$	459.10 0.0	0 66COL/SKI	$\Delta_t G^{\circ} = \ln K_f =$		- 10.78 4.35		
Glutarimide (2×C-(H) ₂ (CO)(C))+(1 (1×N-(H)(CO) ₂)+(1× ₁ Literature - C			Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se 46.70	- 47.55 87.82 169.25 - 129.69 - 8.88 3.58	0.85	61GOO/LAC
Gas phase $\Delta_t H^\circ = -393.60$ -	393.60 0.0	0 90MEN/PIL	Ethanethiol	I			C2HeS
Solid phase $\Delta_t H^\circ = -487.70$ -	487.64 -0.0	6 90MEN/PIL	(1×C-(F		×C-(H)2(C)(S re – Calculated		(H)), σ = 3 Reference
N,N-Bisuccinimide (4×C-(H) ₂ (C)(CO))+(4) (2×succinimide rsc) Literature	4×CO-(C)(N))+(2		Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	-46.11 72.68 296.10	-46.79 72.39 297.73 -137.52 -5.79 2.33	0.68 0.29 ~1.63	52MCC/SCO 69STU/WES 69SYU/WES
Solid phase $\Delta_t H^\circ = -709.36$ —	709.36 0.0	0 66COL/SKI	Liquid phas $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	se - 73.60 117.86 207.02	-74.32 112.00 210.34 -224.91 -7.26 2.93	0.72 5.86 3.32	57MCC/HUB 52MCC/SCO 52MCC/SCO
			1-Propaneth (1×C-(H (1×S-(C	$I_{3}(C) + (1)(H), \sigma =$	\times C-(H) ₂ (C) ₂) 3 e – Calculated		
			Gas phase $\Delta_t H^\circ = C_{t'}^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	-67.86 94.77 336.39	-67.42 95.28 336.89 -234.67 2.55 -1.03	-0.44 -0.51 -0.50	Reference 56PEN/SCO 69STU/WES 69STU/WES

TABLE 42. Thiols (31) - Continued

TABLE 42. Thiols (31) - Continued

(1×C-(H	niol (Contin $I_{3}(C)$) + (1: $I_{3}(C)$), $\sigma =$	\times C-(H) ₂ (C) ₂) +	· (1 × C−(H)₂(C_3H_8S (C)(S))+			\times C-(H) ₂ (C) ₂) = 3	+ (1 × C-(H) ₂	(C)(S) +
	Literatur	e – Calculated =	Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid phas	ie				Gas phase				
$\Delta_{i}H^{\circ} =$	- 99.90	-100.05	0.15	54HUB/WAD	$\Delta_{\rm f}H^{\circ} =$	- 128.99	- 129.31	0.32	66OSB/DOU
$C_p^{\circ} =$	144.56	142.42	2.14	56PEN/SCO	$C_p^{\circ} =$	164.05	163.95	0.10	69STU/WES
S° =	242.50	242.72	-0.22	56PEN/SCO	S° =	454.30	454.37	-0.07	69STU/WES
$\Delta_f S^{\circ} =$		-328.84		n.P	$\Delta_f S^\circ =$		- 526.13		
$\Delta_{\rm f}G^{\circ} =$		- 2.01			$\Delta_t G^{\circ} =$		27.55		
$lnK_f =$		0.81			$lnK_f =$		-11.12		
					Liquid pha	ase			
1-Butaneth	iol			C4H10S	$\Delta_t H^{\circ} =$	-175.70	- 177.24	1.54	66GOO/DEP
(1×C-(H	(C) + (2	\times C-(H) ₂ (C) ₂) +	$+(1\times C-(H)_2)$		$C_p^{\circ} =$	230.71	233.68	-2.97	70FIN/MCC
	$C)(H)), \sigma =$. , /-		S° -	343.21	339.86	3.35	70FIN/MCC
					$\Delta_f S^\circ =$		- 640.63		
	Literatur	re – Calculated =	= Residual	Reference	$\Delta_i G^{\circ} =$		13.76		
					$lnK_f =$		-5.55		
Gas phase $\Delta_t H^\circ =$	- 88.07	- 88.05	-0.02	57SCO/FIN					
$C_p^{\circ} =$	118.16	118.17	-0.02	69STU/WES	1-Heptane	thiol			C7H165
$S^{\circ} =$	375.22	376.05	-0.83	69STU/WES	-		\times C-(H) ₂ (C) ₂)	+ (1 × C-(H)-	
$\Delta_f S^\circ =$	373.22	-331.82	0.05	0,010,1120		$C)(H), \sigma =$		(1 × C=(11)2)	(0)(0)) 1
$\Delta_f G^\circ =$		10.88		,	(1110 (0)(11)), 0	2		
$lnK_f =$		-4.39				Literatu	re – Calculated	= Residual	Reference
			-		-				
Liquid pha		105 50	4.00	#0111 ID/GOO	Gas phase		440.04	0.04	((ODD D OI)
$\Delta_{\rm f}H^{\circ} =$	-124.70	- 125.78	1.08	58HUB/GOO	$\Delta_t H^\circ =$	- 150.00	- 149.94	-0.06	66OSB/DOU
$C_p^{\circ} =$	172.30	172.84	-0.54	57SCO/FIN	$C_p^{\circ} = S^{\circ} =$	186.94	186.84	0.10	69STU/WES
S° = Δ _t S° =	275.98	275.10 - 432.77	0.88	57SCO/FIN	$\Delta_{i}S^{\circ} =$	493.25	493.53 623.28	-0.28	69STU/WES
$\Delta_{\mathbf{f}}G^{\circ} =$		3.25			$\Delta_{\rm f}G^{\circ} =$		35.89		
$lnK_f =$		-1.31			$\ln K_{\rm f} =$		- 14.48		
					Tiouid abo				
1-Pentanet	hiol			C ₅ H ₁₂ S	Liquid pha $\Delta_t H^\circ =$	200.50	-202.97	2.47	66GOO/DEP
		\times C-(H) ₂ (C) ₂)	+ (1 × C-(H)-		$C_p^{\circ} =$	259.32	264.10	- 4.78	70FIN/MCC
	$C)(H)), \sigma =$		· (1 × © (11)2	(0)(0))	$S^{\circ} =$	375.35	372.24	3.11	70FIN/MCC
(1/10/(٥,(٠٠,), ٥	•			$\Delta_f S^\circ =$	570.55	- 744.56	3.11	701 11 711100
	Literatu	re – Calculated:	= Kesidual	Reference	$\Delta_i G^{\circ} =$		19.02		
	25.70				$lnK_f =$		-7.67		
Gas phase	110 10	100 60	1.40	(SEIN/JIOC					
$\Delta_{\rm f}H^{\circ} = C_{\rm p}^{\circ} =$	- 110.10 141.21	108.68 141.06	-1.42 0.15	65FIN/HOS 69STU/WES	1-Octaneth	vial			C ₈ H ₁₈ S
$S^{\circ} =$	415.29	415.21	0.13	69STU/WES			\times C-(H) ₂ (C) ₂)	+ (1 × C-(U).(
$\Delta_{\rm f}S^{\circ} =$	713.67	- 428.97	0.00	07010/4120		$C)(H), \sigma =$. (1 ^ 0=(11)2(~\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
$\Delta_{\rm f}G^{\circ} =$		19.22			(2.00 (~/(*^//)	•		
$lnK_f =$		-7.75				Literatur	re – Calculated	= Residual	Reference
					Gen -1				
T (m. / 4)		151 51	0.50	SALITID/CAT	Gas phase		170 57	0.26	COCTITUTE
Liquid pha	-152.10	-151.51 203.26	-0.59 -2.09	54HUB/CAT 52FINSCO	$\Delta_{\rm f}H^{\circ} =$	- 170.21 209.79	- 170.57 209.73	0.36 0.06	69STU/WES 69STU/WES
$\Delta_{\rm f}H^{\circ} =$	201 17	203.20			$C_p^{\circ} =$				
$\Delta_{f}H^{\circ} = C_{p}^{\circ} =$	201.17 310.37	307 48	7 80	52FIN/SCO	, , , , , , , , , , , , , , , , , , , 	532.20			600111/0/40
$\Delta_t H^\circ = C_p^\circ = S^\circ = S$	201.17 310.37	307.48 536.70	2.89	52FIN/SCO	S° = Λ ₆ S° =	532.20	532.69 720.43	-0.49	69STU/WES
$\Delta_f H^\circ = C_p^\circ =$		307.48 536.70 8.51	2.89	52FIN/SCO	$\Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \Delta_{f}G^{\circ} = 0$	532.20	- 720.43 44.23	- 0.49	69STU/WES

TABLE 42. Thiols (31) - Continued

TABLE 42. Thiols (31) - Continued

	iol (Continued) $H_{3}(C)$) + $(6 \times C - (H)_{2}(C)_{2})$ + $(1 \times C - (H)_{2}(C)_{2})$ (H) , $\sigma = 3$	$C_8H_{18}S$ $(C)(S)) +$			$4 \times C - (H)_2(C)_2$	e) + (1 × C-(H)	$C_{16}H_{34}S_{2}(C)(S)) +$
	Literature - Calculated = Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid pha	se						
$\Delta_i H^\circ =$	- 228.70		Gas phase				
$C_p^{\circ} =$	294.52		$\Delta_{\rm f}H^{\circ} =$	-335.10	-335.61	0.51	69STU/WES
S° =	404.62		$C_p^{\circ} =$	392.75	392.85	-0.10	69STU/WES
$\Delta_{f}S^{\circ} =$	- 848.49		S° =	843.79	845.97	-2.18	69STU/WES
$\Delta_f G^\circ =$	24.28		$\Delta_{\mathbf{f}}S^{\circ} =$		- 1497.64		
$lnK_f =$	- 9.79		$\Delta_f G^\circ = \ln K_f =$		110.91 44.74		
		a ** a					
1-Nonanetl		C ₉ H ₂₀ S	Liquid pha	se	124.54		
	$(H)_3(C) + (7 \times C - (H)_2(C)_2) + (1 \times C - (H)_2)$	(し)(3))+	$\Delta_{f}H^{\circ} =$		- 434.54		
(1 × S-(0	$C(H)$, $\alpha = 3$		$C_{r}^{\circ} = S^{\circ} =$		537.88 663.66		
	Literature - Calculated = Residual	Reference	$\Delta_{f}S^{\circ} =$		- 1679.94		
	Literature - Calculated = Residual	Reference	$\Delta_{\mathbf{f}}G^{\circ} =$		66.33		
			$\ln K_{\rm f} =$		- 26.76		
Gas phase			unt -		20.70		
$\Delta_t H^\circ =$	- 190.83 - 191.20 0.37	69STU/WES					
$C_p^{\circ} =$	232.67 232.62 0.05	69STU/WES					
S° =	571.16 571.85 -0.69	69STU/WES	1-Eicosane	thiol			C ₂₈ H ₄₂ S
$\Delta_f S^\circ =$	~817.58	0,010,			$8 \times C - (H)_2(C)_2$)+(1×C-(H)	
$\Delta_t G^\circ =$	52.56			$C)(H)), \sigma =$, . (2(0)(0)) .
$lnK_f =$	-21.20		(=====	,,(,),, -			
•				Literatui	re – Calculated	= Residual	Reference
Liquid pha							
$\Delta_t H^\circ =$	-254.43		Gas phase				
$C_{\rho}^{\circ} =$	324.94		$\Delta_{\mathbf{f}}H^{\circ} =$	-417.56	-418.13	0.57	69STU/WES
S° =	437.00		$C_p^{\circ} =$	484.26	484.41	- 0.15	69STU/WES
$\Delta_{t}S^{\circ} =$	-952.42		S° =	999.60	1002.61	- 3.01	69STU/WES
$\Delta_!G^\circ =$	29.54		$\Delta_f S^\circ =$		- 1886.24		
$lnK_f =$	-11.91		$\Delta_{f}G^{\circ} =$		144.25		
			$\ln K_{\rm f} =$		-58.19		
1-Decaneth	aiol	CuaHaaS		se	- 58.19 		
1-Decaneth		$C_{10}H_{22}S$	Liquid pha	se			
(1×C-(1	$(H)_3(C) + (8 \times C - (H)_2(C)_2) + (1 \times C - (H)_2)$		Liquid phate $\Delta_t H^\circ =$	se	- 537.46		
(1×C-(1			Liquid pha	se	- 537.46 659.56		
(1×C-(1	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$	(C)(S))+	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ =$	se	- 537.46 659.56 793.18		
(1×C-(1	$(H)_3(C) + (8 \times C - (H)_2(C)_2) + (1 \times C - (H)_2)$		Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = 0$	se	-537.46 659.56 793.18 -2095.67		
(1×C-(1	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$	(C)(S))+	Liquid pha: $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = 0$	se	- 537.46 659.56 793.18 - 2095.67 87.36		
(1 × C-(1) (1 × S-(0)	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$	(C)(S))+	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = 0$	se	-537.46 659.56 793.18 -2095.67		
$(1 \times C - (1 \times S - (0 \times S - (0 \times S + (0 \times S - (0 \times S + (0 \times S - ($	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$	(C)(S))+	Liquid pha: $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = 0$	se	- 537.46 659.56 793.18 - 2095.67 87.36		
(1 × C-(1) (1 × S-(0)	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$ Literature - Calculated = Residual	(C)(S))+ Reference	Liquid pha: $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \Delta_{t}G^{\circ} = 0$	se	- 537.46 659.56 793.18 - 2095.67 87.36		
$(1 \times C - (1 \times S - ($	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$ Literature - Calculated = Residual -211.46 -211.83 0.37 255.56 255.51 0.05 610.11 611.01 -0.90	(C)(S)) + Reference 69STU/WES	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f =$ 1,2-Ethanee	lithiol	- 537.46 659.56 793.18 - 2095.67 87.36 - 35.24		C₂H₄S₂
$(1 \times C - (1 \times S - ($	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$ Literature - Calculated = Residual -211.46 -211.83 0.37 255.56 255.51 0.05	(C)(S)) + Reference 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f =$ 1,2-Ethanee	lithiol	- 537.46 659.56 793.18 - 2095.67 87.36)	C₂H₄S₂
$(1 \times C - (1 \times S - (0 \times S - ($	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$ Literature - Calculated = Residual -211.46 -211.83 0.37 255.56 255.51 0.05 610.11 611.01 -0.90	(C)(S)) + Reference 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f =$ 1,2-Ethanee	lithiol	- 537.46 659.56 793.18 - 2095.67 87.36 - 35.24)	C₂H₄S₂
$(1 \times C - (1 \times S - ($	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$ Literature - Calculated = Residual -211.46 -211.83 0.37 255.56 255.51 0.05 610.11 611.01 -0.90 -914.73	(C)(S)) + Reference 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_f =$ 1,2-Ethanee	lithiol ()(H)) + (2 ×	- 537.46 659.56 793.18 - 2095.67 87.36 - 35.24		C₂H ₆ S₂ Reference
$(1 \times C - (1 \times S - ($	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$ Literature – Calculated = Residual -211.46 -211.83 0.37 255.56 255.51 0.05 610.11 611.01 -0.90 -914.73 60.90 -24.57	(C)(S)) + Reference 69STU/WES 69STU/WES	Liquid pha: $\Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1,2-Ethanee}{2 \times S-(C)}$	lithiol ()(H)) + (2 ×	- 537.46 659.56 793.18 - 2095.67 87.36 - 35.24		
$(1 \times C - (1 \times S - ($	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$ Literature - Calculated = Residual -211.46 -211.83 0.37 255.56 255.51 0.05 610.11 611.01 -0.90 -914.73 60.90 -24.57	(C)(S)) + Reference 69STU/WES 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ 1,2-Ethanee $(2 \times S - (C_0)^2)$ Gas phase	lithiol ()(H)) + (2 × Literatur	- 537.46 659.56 793.18 - 2095.67 87.36 - 35.24 CC-(H) ₂ (C)(S)	= Residual	Reference
$(1 \times C - (1 \times S - ($	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$ Literature - Calculated = Residual -211.46 -211.83 0.37 255.56 255.51 0.05 610.11 611.01 -0.90 -914.73 60.90 -24.57	(C)(S)) + Reference 69STU/WES 69STU/WES	Liquid phat $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ 1,2-Ethanee $(2 \times S - C)$ Gas phase $\Delta_t H^\circ = C_t = C$	lithiol ()(H)) + (2 ×	-537.46 659.56 793.18 -2095.67 87.36 -35.24 c C-(H) ₂ (C)(S) re - Calculated		
$(1 \times C - (1 \times S - ($	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$ Literature - Calculated = Residual -211.46 -211.83 0.37 255.56 255.51 0.05 610.11 611.01 -0.90 -914.73 60.90 -24.57 se -276.50 -280.16 3.66 355.36	(C)(S)) + Reference 69STU/WES 69STU/WES 69STU/WES	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ 1,2-Ethanee $(2 \times S - (C_0)^2)$ Gas phase	lithiol ()(H)) + (2 × Literatur	- 537.46 659.56 793.18 - 2095.67 87.36 - 35.24 CC-(H) ₂ (C)(S)	= Residual	Reference
$(1 \times C - (1 \times S - ($	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$ Literature - Calculated = Residual - 211.46 - 211.83 0.37 255.56 255.51 0.05 610.11 611.01 - 0.90 - 914.73 60.90 - 24.57 se - 276.50 - 280.16 3.66 355.36 469.38	(C)(S)) + Reference 69STU/WES 69STU/WES 69STU/WES	Liquid phat $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ 1,2-Ethanee $(2 \times S - C)$ Gas phase $\Delta_t H^\circ = C_t = C$	lithiol ()(H)) + (2 × Literatur	-537.46 659.56 793.18 -2095.67 87.36 -35.24 c C-(H) ₂ (C)(S) re - Calculated	= Residual	Reference
$(1 \times C - (1 \times S - ($	H) ₃ (C)) + (8 × C-(H) ₂ (C) ₂) + (1 × C-(H) ₂ C)(H)), $\sigma = 3$ Literature - Calculated = Residual -211.46 -211.83 0.37 255.56 255.51 0.05 610.11 611.01 -0.90 -914.73 60.90 -24.57 se -276.50 -280.16 3.66 355.36	(C)(S)) + Reference 69STU/WES 69STU/WES 69STU/WES	Liquid phat $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ 1,2-Ethanee $(2 \times S - C)$ Gas phase $\Delta_t H^\circ = C_t = C$	lithiol ()(H)) + (2 × Literatur	-537.46 659.56 793.18 -2095.67 87.36 -35.24 c C-(H) ₂ (C)(S) re - Calculated	= Residual	Reference

Gas phase $\Delta_l H^\circ = C_p^\circ =$

- 70.95 161.99

TABLE 42. TI	niols (31) — Continu	ed		Table	E 42. Thiols (3)	1) – Continu	ied
1,2-Ethanedithiol (Continued) $(2 \times S-(C)(H)) + (2 \times C-(H))$		C ₂ H ₆ S ₂		edithiol (Co C)(H))+(3>	ontinued) × C–(H) ₂ (C) ₂) +	+ (2 × C-(H) ₂ (C ₅ H ₁₂ ;
Literature – Cal	culated = Residual	Reference			re – Calculated		Reference
Liquid phase	3000						
$C_p^{\circ} =$ 15 $S^{\circ} =$ 25 $\Delta_t S^{\circ} =$ -21 $\Delta_t G^{\circ} =$ 1	3.42 -0.98 11.04 14.08 3.22 0.15 4.10	62MAN/SUN	Liquid pha $ \Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{\ell}S^{\circ} = \Delta_{\ell}G^{\circ} = \ln K_{\ell} = 0 $	se 130.30	- 130.61 242.30 351.22 - 525.01 25.92 - 10.46	0.31	62MAN/SUN
1,3-Propanedithiol (2×S-(C)(H))+(1×C-(H) Literature – Ca) ₂ (C) ₂) + (2 × C~(H) ₂ (culated = Residual	C ₃ H ₈ S ₂ C)(S)) Reference		C)(H))+(2>	< C-(H) ₃ (C)) + iary)), σ = 9	(1×C-(H)(C)	C ₃ H ₈
				Literatur	re – Calculated	= Residual	Reference
	29.69 -0.01 16.21	62MAN/SUN	Gas phase $\Delta_t H^\circ = C_p^\circ =$	-76.23 95.98	- 76.28 97.51	0.05 - 1.53	54MCC/FIN2 69STU/WES
$C_p^{\circ} = 18$ $S^{\circ} = 28$	79.15 - 0.25 81.46 86.46 17.15	62MAN/SUN	$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f = -\infty$	324.30	326.68 - 244.88 - 3.27 1.32	-2.38	69STU/WES
$\ln K_{\rm f} =$	15.41 6.22	CHS	Liquid phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ =$	se - 105.90 145.35 233.55	- 105.59 142.08 235.94 - 335.62	-0.31 3.27 -2.39	54HUB/WAD 54MCC/FIN2 54MCC/FIN2
1,4-Butanedithiol $(2 \times S-(C)(H)) + (2 \times C-(H))$	$(2)_2(C)_2 + (2 \times C - (H)_2)_2$	$C_4H_{10}S_2$ $C)(S))$	$\Delta_f G^\circ = \ln K_f =$		-5.53 2.23		
Literature – Ca	lculated = Residual	Reference					
	50.32 -0.08 39.10	62MAN/SUN		C)(H))+(2×	< C-(H)₃(C)) + - (1 × -CH₃ corr		
				Literatui	re – Calculated	= Residual	Reference
$C_p^{\circ} =$ 2: $S^{\circ} =$ 3: $\Delta_t S^{\circ} =$ -4: $\Delta_t G^{\circ} =$ 2:	04.88 -0.82 11.88 18.84 21.08 20.67 -8.34	62MAN/SUN	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	- 96.90 119.29 366.73	-94.65 120.40 365.84 -342.03 7.33 -2.96	-2.25 -1.11 0.89	58MCC/FIN 69STU/WES 69STU/WES
1,5-Pentanedithiol) (O) \	C ₅ H ₁₂ S ₂			2.70		······································
(2×S-(C)(H)) + (3×C-(H Literature - Ca	$\frac{1}{2}(C)_{2} + (2 \times C - (H)_{2})$ $\frac{1}{2}(C)_{2} + (2 \times C - (H)_{2})$ $\frac{1}{2}(C)_{2} + (2 \times C - (H)_{2})$	Reference	$C_p^{\circ} = S^{\circ} =$	e - 131.00 171.21 266.35	-129.14 172.50 268.32	-1.86 -1.29 -1.97	58HUB/GOO 58MCC/FIN 58MCC/FIN
	70.95 - 0.05 61.99	62MAN/SUN	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-439.55 1.91 -0.77		

TABLE 42. Thiols (31) - Continued

TABLE 42. Thiols (31) - Continued

	$(H) + (1 \times$	ы : C-(H)2(C)(S)] ary)) + (2 × C-((3×C-(I	$H_{3}(C)) + (1$	ol (Continued) l × C-(H)2(C)2) × -CH3 corr (q		
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ - C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ - \ln K_t =$	97.24 118.32 362.88	-94.74 118.20 362.31 -345.56 8.29 -3.34	- 2.50 0.12 0.57	58HUB/GOO 69STU/WES 69STU/WES	Liquid pha $ \Delta_t H^\circ - C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ - \ln K_t = $	se 162.80 198.95 295.60	- 160.59 200.08 281.37 - 562.81 7.21 - 2.91	- 2.21 - 1.13 14.23	62SCO/DOU 74MES/FIN 74MES/FIN
$C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = 0$	ee 132.00 171.88 266.35	-131.06 169.86 269.75 -438.12 -0.43	-0.94 2.02 -3.40	58SCO/MCC 58SCO/MCC 58SCO/MCC		C)(H))+(2: H) ₂ (C) ₂)+(l × C-(H) ₃ (C)) + 1 × C-(H)(C) ₃) re – Calculated	+(2×-CH ₃ c	
	(H))+(3×	(C-(H) ₃ (C))+		C₄H ₁₀ S	Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 114.90	-115.37 141.09	0.47	72GOO2
(3×-CH		re – Calculated		Reference	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ =$	se - 154.30 200.33 298.49	-156.79 200.28 302.13	2.49 0.05 -3.64	72GOO2 74MES/FIN 74MES/FIN
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	-109.60 120.96 338.02	-108.30 119.97 337.71 -370.16	-1.30 0.99 0.31	53MCC/SCO 69STU/WES 69STU/WES	$\Delta_{f}S^{\circ} = \\ \Delta_{f}G^{\circ} = \\ \ln K_{f} = $		-542.05 4.82 -1.95		
$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = \\ -$		2.06 - 0.83				(1)(H))+(1	\times C-(H)(C) ₂ (S); sub) rsc), $\sigma = 1$		C ₅ H ₁₀ S ₂ (C) ₂) +
Liquid phase $\Delta_t H^\circ = C_{t'} = C_{t'}$	-140.50 175.06	-139.25 169.66	-1.25 5.40	58HUB/GOO 53MCC/SCO		•	re – Calculated		Reference
$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f =$	246.44	248.99 -458.88 -2.44 0.98	- 2.55	53MCC/SCO	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	-47.91 107.91 361.41	- 50.21 109.74 365.34	2.30 - 1.83 - 3.93	61BER/SCO 69STU/WES 69STU/WES
(3×C-(I	/- \ // \	\times C-(H) ₂ (C) ₂)	, , , , ,	"	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-348.27 53.63 -21.63		
(1×C-(0		×-CH ₃ corr (q	• 77.	Reference	Liquid phas $ \Delta_t H^\circ - C_\rho^\circ = $	se - 89.50 165.23	- 85.34 167.48	4.16 2.25	61BER/SCO 61BER/SCO
Gas phase $\Delta_r H^\circ = C_\rho^\circ = S^\circ =$	-127.03 143.51 386.94	- 124.37 142.86 376.87	- 2.66 0.65 10.07	62SCO/DOU 69STU/WES 69STU/WES	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = -\infty$	256.86	255.51 - 458.10 51.24 - 20.67	1.35	61BER/SCO
$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-467.31 14.96 -6.03							·

TABLE 42. Thiols (31) - Continued

TABLE 42. Thiols (31) - Continued

	Literature	- Calculated	= Residual 	Reference	Literat	ure – Calculated = Residua	al Reference
as phase					Gas phase		
Δ _t H° =	-96.10	- 90.78	-5.32	72GOO2	$\Delta_{\rm f}H^{\rm o}=-115.10$	-113.11 -1.99	72GOO2
C _p =		137.68			C _p =	141.09	
iquid phas	se				Liquid phase		
	- 140.70	- 136.72	-3.98	72GOO2	$\Delta_t H^\circ = -154.40$	-154.61 0.21	72GOO2
$C_p^{\circ} =$	192.63	195.01	-2.38	67MES/TOD	$C_p^{\circ} =$	200.28	
S* =	258.57	256.34	2.23	67MES/TOD	<i>S</i> * =	302.13	
$\Delta_f S^\circ =$		-593.58			$\Delta_f S^\circ =$	-542.05	
$\Delta_t G^\circ =$		40.26			$\Delta_i G^{\circ} =$	7.00	
$lnK_f =$		-16.24			$lnK_f =$	-2.82	
(3×C-(I				C ₅ H ₁₂ S rr (tertiary)) + corr (tertiary))		ethiol (1 × C-(H)(C) ₃) + (2 × -CH 1 × C-(C) ₃ (S)) + (1 × -CH ₃	
(, , ,,	- Calculated		Reference		ure – Calculated = Residua	
Gas phase					Gas phase		
$\Delta_i H^\circ =$	- 121.30	- 121.97	0.67	72GOO2	$\Delta_t H^\circ = -147.90$	-144.37 -3.53	72GOO2
$C_p^{\circ} =$	-121.50	143.32	0.07	720002	$C_p^o =$	165.78	720002
Liquid pha					Liquid phase		
aquia pila Δ _i H° =	158.80	- 160.15	1.35	72GOO2	$\Delta_t H^\circ = -187.20$	-184.59 -2.61	72GOO2
$C_p^{\circ} =$	150.00	199.94			$C_p^{\circ} =$	227.52	
S° =		295.35			S° =	308.40	
Δ _f S° =		-548.83			$\Delta_{f}S^{\circ} =$	- 672.09	
$\Delta_{\rm f} G^{\circ} =$		3.48			$\Delta_t G^{\circ} =$	15.79	
$lnK_f =$		-1.41			$lnK_f =$	- 6.37	· · · · · · · · · · · · · · · · · · ·
					2-Methyl-2-pentaneth		Cal
(3×C-(1	hyl-1-propane H) ₃ (C)) + (1: H) ₂ (C)(S)) +		×-CH3 corr (C₅H ₁₂ S quaternary))+	$(3 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)_2) +$	$(1 \times C - (C)_3(S)) + (2 \times -CH_3)$	-
(3×C-(1	H) ₃ (C))+(1: H) ₂ (C)(S))+	\times C-(C) ₄) + (3)		$(2 \times C - (H)_2(C)_2) +$	$(1 \times C - (C)_3(S)) + (2 \times -CH_3)$	corr (quaternary))
(3×C-(1) (1×C-(1)	$(H)_3(C) + (1:H)_2(C)(S) + (1:H)_2(C)(S)$	× C-(C) ₄) + (3 (1 × S-(C)(H) e – Calculated) = Residual	quaternary)) + Reference	(2×C-(H) ₂ (C) ₂)+ Literate Gas phase	$(1 \times C - (C)_3(S)) + (2 \times -CH_3)$ $(1 \times S - (C)(H))$ ure - Calculated = Residua	corr (quaternary)
$(3 \times C - (1 \times C + ($	H)₃(C)) + (1: H)₂(C)(S)) + Literatur	× C-(C) ₄) + (3 (1 × S-(C)(H) e - Calculated - 125.79)	quaternary))+	$(2 \times C - (H)_2(C)_2) +$ Literate Gas phase $\Delta_t H^\circ = -148.30$	$(1 \times C - (C)_3(S)) + (2 \times -CH_3)$ $(1 \times S - (C)(H))$ ure - Calculated = Residua -145.00 - 3.30	corr (quaternary)
(3×C-(1) (1×C-(1)	$(H)_3(C) + (1:H)_2(C)(S) + (1:H)_2(C)(S)$	× C-(C) ₄) + (3 (1 × S-(C)(H) e – Calculated) = Residual	quaternary)) + Reference	(2×C-(H) ₂ (C) ₂)+ Literate Gas phase	$(1 \times C - (C)_3(S)) + (2 \times -CH_3)$ $(1 \times S - (C)(H))$ ure - Calculated = Residua	corr (quaternary)
$(3 \times C - (1 \times C))))))))))))))))))))$	H) ₃ (C)) + (1: H) ₂ (C)(S)) + Literatur - 129.00	× C-(C) ₄) + (3 (1 × S-(C)(H) e - Calculated - 125.79) = Residual	quaternary)) + Reference	$(2 \times C - (H)_2(C)_2) +$ Literate Gas phase $\Delta_t H^\circ = -148.30$	$(1 \times C - (C)_3(S)) + (2 \times -CH_3)$ $(1 \times S - (C)(H))$ ure - Calculated = Residua -145.00 - 3.30	corr (quaternary) Reference
$(3 \times C - (1 \times C)))))))))))))))))))$	H) ₃ (C)) + (1: H) ₂ (C)(S)) + Literatur - 129.00	× C-(C) ₄) + (3 (1 × S-(C)(H) e - Calculated - 125.79) = Residual	quaternary)) + Reference	$(2 \times C - (H)_2(C)_2) +$ Literate Gas phase $\Delta_t H^{\circ} = -148.30$ $C_p^{\circ} =$	$(1 \times C - (C)_3(S)) + (2 \times -CH_3)$ $(1 \times S - (C)(H))$ ure - Calculated = Residua -145.00 - 3.30	Reference
$(3 \times C - (1 \times C + ($	H) ₃ (C)) + (1: H) ₂ (C)(S)) + Literatur - 129.00	×C-(C) ₄) + (3 (1×S-(C)(H)) e - Calculated -125.79 140.38	-3.21	quaternary)) + Reference 72GOO2	$(2 \times C - (H)_2(C)_2) +$ Literate Gas phase $\Delta_t H^\circ = -148.30$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = -188.30$	$(1 \times C - (C)_3(S)) + (2 \times -CH_3)$ $(1 \times S - (C)(H))$ ure - Calculated = Residua - 145.00 - 3.30 165.75 186.32 - 1.98	I Reference 72GOO2
$(3 \times C - (1 \times C)))))))))))))))))))$	H) ₃ (C)) + (1: H) ₂ (C)(S)) + Literatur - 129.00	×C-(C) ₄) + (3 (1×S-(C)(H)) e - Calculated -125.79 140.38 -164.72 195.20	-3.21	quaternary)) + Reference 72GOO2	$(2 \times C - (H)_2(C)_2) +$ Literate Gas phase $\Delta_t H^\circ = -148.30$ $C_p^\circ =$ Liquid phase	$(1 \times C - (C)_3(S)) + (2 \times -CH_3)$ $(1 \times S - (C)(H))$ ure - Calculated = Residua - 145.00 - 3.30 165.75 186.32 - 1.98 230.50	I Reference 72GOO2
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid pha $\Delta_t H^\circ = C_p^\circ = S^\circ =$	H) ₃ (C)) + (1: H) ₂ (C)(S)) + Literatur - 129.00	×C-(C) ₄) + (3 (1×S-(C)(H)) e - Calculated - 125.79 140.38 - 164.72 195.20 278.29	-3.21	quaternary)) + Reference 72GOO2	$(2 \times C - (H)_2(C)_2) +$ Literate Gas phase $\Delta_t H^\circ = -148.30$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = -188.30$ $C_p^\circ =$ $S^\circ =$	$(1 \times C - (C)_3(S)) + (2 \times -CH_3)$ $(1 \times S - (C)(H))$ ure - Calculated = Residua - 145.00 - 3.30 165.75 186.32 - 1.98 230.50 313.75	Reference
$(3 \times C - (1 \times C))))))))))))))))))$	H) ₃ (C)) + (1: H) ₂ (C)(S)) + Literatur - 129.00	×C-(C) ₄) + (3 (1×S-(C)(H)) e - Calculated -125.79 140.38 -164.72 195.20	-3.21	quaternary)) + Reference 72GOO2	$(2 \times C - (H)_2(C)_2) +$ Literate Gas phase $\Delta_t H^\circ = -148.30$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = -188.30$ $C_p^\circ =$	$(1 \times C - (C)_3(S)) + (2 \times -CH_3)$ $(1 \times S - (C)(H))$ ure - Calculated = Residua - 145.00 - 3.30 165.75 186.32 - 1.98 230.50	Reference 72GOO2

TABLE 42. Thiols (31) - Continued

TABLE 43. Sulfides (32)

Benzenethio (1 × S–(C		< C _B -(S)) + (5×	$C_B-(H)(C_B)$	C_6H_6S ₂), $\sigma = 2$	Dimethyl so (2×C-(I		×S-(C) ₂), σ =	: 18	C₂H ₆
	Literature	e – Calculated =	Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	112.40 104.89 336.85	112.40 104.89 336.85 - 121.36 148.58	0.00 0.00 0.00	56SCO/MCC 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	-37.53 74.10 285.80	-37.53 74.10 285.80 -149.45 7.03	0.00 0.00 0.00	57MCC/HUB 69STU/WES 69STU/WES
$lnK_f =$		- 59.94			$lnK_f =$		- 2.84		
Liquid phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	63.70 173.22 222.80	63.70 173.22 222.80 - 235.41 133.89 - 54.01	0.00 0.00 0.00	56SCO/MCC 56SCO/MCC 56SCO/MCC	Liquid phas $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	se -65.40 118.11 196.40	-65.40 118.11 196.40 -238.85 5.81 -2.34	0.00 0.00 0.00	57MCC/HUB 42OSB/DOE 42OSB/DOE
	C)(H))+(1× (H)(C _B) ₂)	$C-(H)_2(C_B)(S)$ e – Calculated =		C_7H_8S $C)(C_B)_2) +$ Reference	Ethyl methy (1×C-(F (1×S-(C	$(1)_3(C) + (1)_2$, $\sigma = 9$	× C-(H)3(S)) + re – Calculated		C ₃ H _e C)(S)) + Reference
Gas phase $\Delta_t H^\circ =$	92.80	92.80	0.00	72GOO2	Gas phase $\Delta_t H^\circ = C_\rho^\circ =$	-59.62 95.10	- 60.70 95.00	1.08 0.10	51SCO/FIN 69STU/WES
Liquid pha Δ _f H° =	se 36.20	36.20	0.00	72GOO2	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} =$	333.10	333.43 -238.13 10.30 -4.15	-0.33	69STU/WES
					Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se 91.60 144.64 239.00	-92.17 142.29 237.49 -334.07 7.43 -3.00	0.57 2.35 1.51	54HUB/WAD 51SCO/FIN 51SCO/FIN
					Diethyl sulf (2×C-(H	fide 1)3(C))+(2	× C-(H)2(C)(S))+(1×S-(C)	$C_4H_{10}S_{2}$, $\sigma = 18$
						Literatur	e – Calculated	= Residual	Reference
					Gas phase $ \Delta_t H^\circ = C_\rho^\circ = S^\circ - \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0 $	- 83.74 117.03 368.00	-83.87 115.90 369.54 -338.33 17.00 -6.86	0.13 1.13 -1.54	52SCO/FIN2 69STU/WES 69STU/WES

TABLE 43.	Sulfides	(32) -	Continued
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TABLE 43.	Sulfides	(32) -	Continued
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(2×C-(H	ide (Contina () ₃ (C)) + (2 >	1 ed) < C-(H)2(C)(S)))+(1×S-(C)	$C_4H_{10}S$ $\rho_2), \sigma = 18$		$H)_3(C)) + (2$	$\times C - (H)_2(C)_2$ + $(1 \times S - (C)_2)$,		C ₅ H ₁₂ (S)) +
	Literature	e – Calculated	= Residual	Reference	(11.0)		re – Calculated		Reference
Liquid phas	20								
	119.40 171.42 269.28	118.94 166.47 278.58	-0.46 4.95 -9.30	58HUB/GOO 52SCO/FIN2 52SCO/FIN2	Gas phase $\Delta_f H^\circ = C_p^\circ =$	- 102.17 140.75	- 101.96 140.78	-0.21 -0.03	61MCC/FIN 69STU/WES
$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-429.29 9.05 -3.65			$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f =$	411.80	411.75 -432.43 26.97 -10.88	0.05	69STU/WES
sopropyl n	nethyl sulfid	e		C ₄ H ₁₀ S	Liquid pha	ise			
		× C-(H)3(S))+ CH3 corr (tertia			$\Delta_t H^\circ = C_p^\circ = S^\circ =$	- 142.90 200.92 307.48	-143.63 203.13 302.25	0.73 -2.21 5.23	61MCC/FIN 61MCC/FIN 61MCC/FIN
	Literatur	e – Calculated	= Residual	Reference	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-541.93 17.95 -7.24		
Gas phase $\Delta_t H^\circ =$	-90.42	- 90.19	-0.23	55MCC/FIN				·	
$C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = $	117.15 359.30	120.12 362.39 -345.48 12.82	2.97 3.09	69STU/WES 69STU/WES			× C-(H) ₂ (C) ₂)	+ (2×C-(H) ₂	C ₅ H ₁₂ (C)(S)) +
$lnK_f =$	<u> </u>	-5.17				Literatur	re – Calculated	= Residual	Reference
Liquid pha $ \Delta_t H^\circ = C_p^\circ = $	se - 124.70 172.38	- 123.44 172.37	- 1.26 0.01	58HUB/GOO 55MCC/FIN	Gas phase $\Delta_t H^\circ =$	- 104.60	- 104.50	-0.10	61MCC/FIN
$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = 0$	263.09	263.09 - 444.78 9.17 - 3.70	0.00	55MCC/FIN	$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = 0$	139.12 414.10	138.79 414.46 -429.72 23.62	0.33 -0.36	69STU/WES 69STU/WES
	ppyl sulfide H) ₃ (C))+(1	× C-(H)3(S)) +	- (1×C-(H) ₂ (C ₄ H ₁₆ S	$lnK_f =$ Liquid pha $\Delta_t H^\circ =$	use - 144.80	- 9.53 - 144.67	-0.13	61MCC/FIN
	H) ₂ (C)(S)) +	$(1 \times S - (C)_2)$, o	r = 9		$C_p^{\circ} = S^{\circ} =$	198.41 309.53	196.89 310.96	1.52 -1.43	61MCC/FIN 61MCC/FIN
	Literatu	e – Calculated	= Residual	Reference	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$		-533.22 14.31 -5.77		
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \Delta_t G^\circ = S^\circ = $	-81.76 117.36 371.70	-81.33 117.89 372.59 -335.28 18.63	- 0.43 - 0.53 - 0.89	57SCO/FIN 69STU/WES 69STU/WES	Butyl ethyl		× C-(H) ₂ (C) ₂)	+ (2 × C-(H) ₂ (C ₆ H ₁₄ (C)(S)) +
$lnK_f =$		-7.52				Literatur	re – Calculated	= Residual	Reference
Liquid phate $\Delta_{i}H^{\circ} =$	nse - 118.50	117.90	- 0.60	58HUB/GOO	Gas phase				
$C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = 0$	171.63 272.54	172.71 269.87 - 438.00 12.69	- 1.08 2.67	57SCO/FIN 57SCO/FIN	$\Delta_t H^\circ = C_p^\circ = S^\circ - \Delta_t S^\circ =$	- 125.19 161.96 453.00	-125.13 161.68 453.62 -526.87	- 0.06 0.28 - 0.62	62MAC/MAY 69STU/WES 69STU/WES

	sulfide (Cos (C_3)) + (2 (C_2)), $\sigma = 9$	ntinued) \times C-(H) ₂ (C) ₂)	+ (2×C-(H) ₂ ($C_6H_{14}S$ $(C)(S)) +$			$X \times C - (H)_2(C)_2$	+ (2 × C-(H) ₂ ((C)(S) +
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid phas	e				Gas phase				
	- 172.30	- 170.40	- 1.90	62MAC/MAY	$\Delta_c H^{\circ} =$	- 125.35	- 125.13	-0.22	61MCC/FIN
$C_p^{\circ} =$		227.31	•		$C_p^{\circ} =$	161.21	161.68	-0.47	69STU/WES
S° =		343.34			S° ==	448.36	447.86	0.50	69STU/WES
$\Delta_f S^\circ =$		-637.15			$\Delta_f S^\circ =$		-532.63		
$\Delta_{\mathbf{f}}G^{\circ} - \\ \ln K_{\mathbf{f}} =$		19.57 - 7.89			$\Delta_t G^\circ = \ln K_t =$		33.67 13.58		
								······································	
					Liquid pha				
Diisopropyl				$C_6H_{14}S$	$\Delta_t H^\circ =$	-169.90	- 170.40	0.50	61MCC/FIN
		\times C-(H)(C) ₂ (S			$C_p^{\circ} =$	225.48	227.31	-1.83	61MCC/FIN
(4×-CH	corr (terti	ary))+(1×S-($(C)_2$, $\sigma = 162$	4	S° =	338.28	343.34	~ 5.06	61MCC/FIN
	T 14 .		_ D!d!	D of ones:	$\Delta_f S^\circ =$		-637.15		
	Literatui	e – Calculated	= Residuai	Reference	$\Delta_t G^\circ = \ln K_t =$		19.57 7.89		
Gas phase									
$\Delta_t H^\circ =$	- 141.25	- 142.85	1.60	62MAC/MAY					
$C_p^{\circ} =$	169.24	166.14	3.10	69STU/WES	Butyl propy	yl sulfide			C7H16
S° =	415.47	427.45	- 11.98	69STU/WES			\times C-(H) ₂ (C) ₂)	+ (2 × C-(H))	
Δ _r S° -		-553.04		,		$(2)_2$, $\sigma = 9$	- (/2(-/2)	(-/(-//
$\Delta_f G^\circ =$		22.04				- /			
$lnK_f =$		-8.89				Literatu	re – Calculated	= Residual	Reference
Liquid phas		101 40	0.12	62MAC/MAY	Gas phase $\Delta_t H^\circ =$	145.04	145 76	0.10	COCTI INVICE
$\Delta_t H^\circ =$	-181.60 232.00	-181.48 226.63	-0.12 5.37	62MAC/MAY 67MES/TOD	-	- 145.94 184.05	- 145.76 184.57	-0.18	69STU/WES
$C_p^{\circ} = S^{\circ} =$	313.05	329.78	- 16.73	67MES/TOD	$C_p^{\circ} = S^{\circ} =$	493.95	492.78	-0.52 1.17	69STU/WES
$\Delta_f S^\circ =$	313.03	-650.71	10.75	O/MEG/10D	$\Delta_t S^\circ =$	475.75	- 624.02	1.17	69STU/WES
$\Delta_f G^\circ =$		12.53			$\Delta_{\rm f}G^{\circ} =$		40.29		
$lnK_f =$		-5.05			$\ln K_{\rm f} =$		-16.25		
Methyl pen	tul multida			C ₆ H ₁₄ S	Liquid phas $\Delta_t H^\circ =$	se	-196.13		
	•	\times C-(H) ₂ (C) ₂)	+ (1 × C-(H)-)		$C_{\rho}^{\circ} =$		257.73		
		$(1 \times S - (C)_2)$		3))+	S° =		375.72		
(1 > C (1	1/2(0)(0))	(1 ~ 0 (0)2), (, ,		$\Delta_{f}S^{\circ} =$		-741.08		
	Literatu	e – Calculated	= Residual	Reference	$\Delta_t G^{\circ} =$		24.82		
					$lnK_f =$		- 10.01		
Gas phase									
$\Delta_{\rm f} H^{\circ} =$	- 122.76	-122.59	-0.17	62MAC/MAY					
$C_p^{\circ} =$	163.59	163.67	-0.08	69STU/WES	Ethyl penty	l sulfide			C7H16S
S° =	450.74	450.91	-0.17	69STU/WES	(2×C-(I	$H_{3}(C) + (3$	\times C-(H) ₂ (C) ₂)	$+(2\times C-(H)_2($	
$\Delta_f S^\circ =$		- 529.58			(1×S-(C	$(2)_2$, $\sigma = 9$			
$\Delta_f G^\circ =$		35.30							•
lnK _t =		- 14.24				Literatus	re – Calculated	- Residual	Reference
					·				
Liquid pha		460.00		(0) (1) (0) (1)	Gas phase	4.45.00			
$\Delta_t H^\circ -$	-167.10	- 169.36	2.26	62MAC/MAY	$\Delta_{\rm r}H^{\circ}$ –	- 145.81	- 145.76	- 0.05	69STU/WES
$C_p^{\circ} =$		233.55			$C_p^{\circ} =$	184.84	184.57	0.27	69STU/WES
		334.63			S° =	491.95	492.78	-0.83	69STU/WES
S° =		645.86			$\Delta_f S^\circ =$		- 624.02		
$\Delta_f S^\circ =$. ~ -				
		23.20 - 9.36			$\Delta_t G^\circ = \ln K_t =$		40.29 - 16.25		

TABLE 43. Sulfides (32) - Continued

	$(1)_3(C) + (3 \times C - (H)_2(G)_2), \ \sigma = 9$	C)2) + (2 × C (11)2	(0)(0)) !		5-(C) ₂)		x = (C)3(O)) 1	(or cris co.	rr (quat/quat))+
	Literature – Calcul	ated = Residual	Reference			Literatu	re – Calculated	= Residual	Reference
Liquid phas	se .			Gas ph	ase				
$\Delta_t H^{\circ} =$	- 196.1	3		$\Delta_f H^\circ =$		188.90	- 183.37	-5.53	62MAC/MAY
$C_p^{\circ} =$	257.7	3		$C_p^o =$	=		211.06		
s° =	375.7	2							
$\Delta_f S^\circ =$	-741.0	8							
$\Delta_f G^\circ =$	24.8			Liquid	phase				
$lnK_f =$	-10.0	1		$\Delta_f H^\circ =$		232.60	-226.30	-6.30	62MAC/MAY
				$C_p^{\circ} =$			281.79		
				S° =			355.88		
		4		Δ _f S° =			-897.23		
Diisobutyl s	sulfide		C ₈ H ₁₈ S	$\Delta_f G^\circ =$			41.21		
(4 × C(F	$H_{3}(C) + (2 \times C - (H))(4)$ $H_{2}(C)(S) + (1 \times S - (C))$			lnK _f =			-16.62		···
	Literature – Calcu	lated = Residual	Reference	**		.e			a w .
				Hexyl n	•		C (II) (C))	. (1) (7 (7)	C ₇ H ₁₆ S
C				(1 × 0	~(n) ₃	(0))+(4	\times C-(H) ₂ (C) ₂	+ (1 × C-(H)2	(C)(3))+
Gas phase	170.50 170.5		COMACIMAN	(1 X S	5-(C) ₂))+(1×C	$-(H)_3(S)), \sigma =$	9	
	-179.50 -179.7		62MAC/MAY			T	01111	n	D (
$C_p^{\circ} =$	207.5					Literatu	re – Calculated	= Residual	Reference
Liquid phas				Gas ph			•		
•	-229.20 -232.4		62MAC/MAY	$\Delta_{\rm f}H^{\circ} =$		145.27	-143.22	- 2.05	62MAC/MAY
$C_p^{\circ} =$	282.1	9		$C_p^{\circ} =$		186.48	186.56	- 0.08	69STU/WES
S° =	397.4	Ю		S° =		489.70	490.07	- 0.37	69STU/WES
$\Delta_{\mathbf{f}}S^{\circ} =$	-855.7	' 1		$\Delta_{\rm f} S^{\circ} =$			- 626.73		
$\Delta_l G^\circ =$	22.7	71		$\Delta_i G^\circ =$	=		43.64		
$lnK_f =$	9,1			$lnK_f =$	-		- 17.60		
				Liquid ;					
Diisopentyl			$C_{10}H_{22}S$	$\Delta_{\rm f}H^{\circ}$ =		190.46	- 195.09	4.63	62MAC/MAY
	H)₃(C))+(2×C–(H)(C_p° =			263.97		
(2×C-(I	$H_{2}(C)_{2} + (2 \times C - (H))_{2}$	$_{2}(C)(S))+(1\times S-(C)(S))$	$\mathbb{C})_2)$	S° =			367.01		
				Δ _f S° =			- 749.79		
	Literature – Calcu	lated≔ Residual	Reference	$\Delta_t G^{\circ} =$	=		28.46		
				$lnK_f =$			-11.48		
Gas phase									
$\Delta_{\mathbf{f}}H^{\circ} =$	-221.50 -221.0		62MAC/MAY						
$C_p^{\circ} =$	253.3	30		Dibutyl	sulfid	e			C ₈ H ₁₈ S
				(2×0	C-(H)3	(C))+(4	\times C-(H) ₂ (C) ₂)	$+(2\times C-(H)_2)$	(C)(S))+
				(1×5	S-(C) ₂)	$\sigma = 18$	3		
Liquid pha									
$\Delta_t H^\circ =$	-281.80 -283.8	38 2.08	62MAC/MAY			Literatu	re – Calculated	= Residual	Reference
$C_p^{\circ} =$	343.0								<u> </u>
S° =	462.1								
$\Delta_f S^\circ =$	- 1063.			Gas ph					
$\Delta_f G^{\circ} =$	33.1	22		$\Delta_{\rm f}H^{\circ}$ =		167.32	-166.39	~ 0.93	61MCC/FIN
$lnK_f =$	- 13.4	1 0		$C_p^{\circ} =$	= :	206.94	207.46	-0.52	69STU/WES
				S° =	= .	526.52	526.18	0.34	69STU/WES
				$\Delta_f S^\circ =$			- 726.93		
				$\Delta_f G^\circ =$			50.35		
				$lnK_f =$			-20.31		
				nus; -			20.31		

TABLE 43. Sulfides (32) - Continued

(2×C-(F	fide (Contin $f(C)$) + (4 $f(C)$), $\sigma = 18$	\times C-(H) ₂ (C) ₂) +	-(2×C-(H) ₂	$C_8H_{18}S$ (C)(S))+			5×C-(H) ₂ (C) ₂)	+ (2×C-(H) ₂	$C_{10}H_{22}S$ (C)(S)) +
	Literatur	e – Calculated =	Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid phas	se				Gas phase				
$\Delta_t H^\circ =$	-220.70	-221.86	1.16	61MCC/FIN	$\Delta_f H^\circ =$	- 208.53	-207.65	-0.88	62MAC/MAY
$C_p^{\circ} =$	284.34	288.15	-3.81	61MCC/FIN	$C_p^{\circ} =$	252.67	253.24	-0.57	69STU/WES
S° =	405.09	408.10	-3.01	61MCC/FIN	S° =	604.38	604.50	-0.12	69STU/WES
$\Delta_f S^\circ =$		- 845.01			$\Delta_{\rm f}S^{\circ} = 0$		-921.24		
$\Delta_f G^\circ = \ln K_f =$		30.08 12.13			$\Delta_t G^\circ = \ln K_t =$		67.02 27.03		
									
					Liquid pha	se			
Ethyl hexyl	sulfide			$C_8H_{18}S$	$\Delta_f H^\circ =$	-266.40	-273.32	6.92	62MAC/MAY
		\times C-(H) ₂ (C) ₂)+	$-(2\times C-(H)_2$	(C)(S))+	$C_p^{\circ} =$		348.99		
	$C)_2), \sigma = 9$. ,		S° =		472.86		
, ,					$\Delta_{f}S^{\circ} =$		- 1052.88		
	Literatur	e – Calculated =	= Residual	Reference	$\Delta_t G^\circ =$		40.59		
					$lnK_f =$		- 16.38		
Gas phase	466.10	466.00	0.04	COCTILATIO					
$\Delta_{\rm f}H^{\circ} =$	-166.40	- 166.39	-0.01	69STU/WES	mark 3 to 1	116" ?			
$C_p^{\circ} \approx$	207.69	207.46	0.23	69STU/WES	Butyl hepty		1a (II) (0) \		C ₁₁ H ₂₄ S
S° =	530.91	531.94	-1.03	69STU/WES			$V \times C - (H)_2(C)_2$	$+(2\times C-(H)_2)$	(C)(S))+
$\Delta_{t}S^{n} =$		-721.17			(1×5-(C	$C)_2), \sigma = 9$			
$\Delta_i G^\circ =$		48.63				Y !4	0-11-41	D	D 0
$lnK_f =$		- 19.62				Literatu	re – Calculated	= Residual	Reference
Liquid pha	ise				Gas phase				
$\Delta_t H^\circ =$		- 221.86			$\Delta_t H^\circ =$	-229.16	-228.28	- 0.88	69STU/WES
$C_p^{\circ} =$		288.15			$C_p^{\circ} =$	275.56	276.13	- 0.57	69STU/WES
S° =		408.10			S° =	649.11	649.42	-0.31	69STU/WES
$\Delta_f S^\circ =$		- 845.01			$\Delta_{f}S^{\circ} =$		- 1012.62	0.01	0,010,1120
$\Delta_{\mathbf{f}}G^{\circ} =$		30.08			$\Delta_{\mathfrak{l}}G^{\circ} =$		73.63		
$lnK_f =$		- 12.13			$lnK_f =$		-29.70		
				· 1879 1879 1879 1879 1879 1879 1879 1879 1879 1879 1879 1879 1879 187			····		
					Liquid phas	se			
	thyl sulfide		(46. (11)	C ₈ H ₁₈ S	$\Delta_f H^\circ =$		- 299.05		
(1×C-(1	H) ₃ (C)) + (5	× C-(H) ₂ (C) ₂) +	F(1×C-(H)2	(C)(S))+	$C_p^{\circ} =$		379.41		
(1×5-(0	$C)_2)+(1\times C)_2$	$-(H)_3(S)), \sigma =$	y		S° =		.505.24		
		0.111	Deside of	D - C	$\Delta_{\rm f} S^{\circ} =$		- 1156.81		
	Literatui	re – Calculated =	= Residual	Reference	$\Delta_{\mathbf{f}}G^{\circ} = \ln K_{\mathbf{f}} =$		45.85 18.50		
0 - 1						<u>-</u>			
Gas phase		162 05	_0.12	COSTILATES					
$\Delta_t H^\circ =$	-163.97	- 163.85	-0.12	69STU/WES	Dit.	es.			
$C_p^{\circ} =$	209.33	209.45	-0.12	69STU/WES	Dihexyl sul		~ (B) (O) \	1040 m	C ₁₂ H ₂₆ S
S° =	528.65	529.23 - 723.88	-0.58	69STU/WES			\times C-(H) ₂ (C) ₂)	+ (∠ × U~(H) ₂ ((C)(3))+
$\Delta_{\rm f}S^{\circ} =$					(1 × 2-(C	$C)_2), \sigma = 18$	3		
$\Delta_l G^{\circ} =$		51.98				T	0.1 1	ъ	5 .0
$lnK_f =$		- 20.97				Literatu	re — Calculated	- Residual	Reference
	ase.	-			Gas phase				
Liquid aka	200	- 220.82	•		$\Delta_r H^\circ =$	- 249.74	- 248.91	- 0.83	69STU/WES
Liquid pha		- 220.02			$C_p^{\circ} =$	298.40	- 248.91 299.02	-0.83 -0.62	69STU/WES
$\Delta_1 H^{\circ} =$		204 30			Up -	47U.TU	477.04	- 0.02	U731U/WE3
$\Delta_r H^\circ = C_p^\circ =$		294,39 300 30				682.28	682 83	D 54	
$\Delta_{r}H^{\circ} = C_{p}^{\circ} = S^{\circ} =$		399.39		•	S° =	682.28	682.82	-0.54	69STU/WES
$\Delta_{r}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = C_{p}^{\circ}$		399.39 -853.72			$S^{\circ} = \Delta_{f}S^{\circ} =$	682.28	- 1115.54	-0.54	
$\Delta_r H^\circ = C_p^\circ = S^\circ =$		399.39			S° =	682.28		- 0.54	

TABLE 43. Sulfides (32) - Continued

TABLE 43.	Sulfides (32)	 Continued

	e (Continued) (C)) + $(8 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(C)_2) $	$(H)_2(C)(S)$ +		(C) + (1			C ₅ H ₁₂ : + (1 × C-(C) ₃ (S)) +
	Literature – Calculated = Residua	al Reference	(3×-cn		ernary)), $\sigma =$		Reference
Liquid phase							
$\Delta_t H^\circ =$	-324.78		Gas phase				
$C_p^{\circ} =$	409.83		$\Delta_{\rm f}H^{\circ} =$	- 121.04	- 122.21	1.17	62SCO/GOO
$S^{\circ} =$	537.62		$C_p^{\circ} =$	145.02	142.58	2.44	69STU/WES
$\Delta_f S^\circ =$	- 1260.74		$S^{\circ} =$	373.25	373.42	-0.17	
				313.43	-470.76	-0.17	69STU/WES
$\Delta_{\rm f}G^{\circ} =$	51.11		$\Delta_f S^\circ =$				
$lnK_f =$	- 20.62		$\Delta_{\rm f}G^{\circ} =$		18.15		
			$lnK_f =$		-7.32		
Butyl nonyl s	ulfide	$C_{13}H_{28}S$	Liquid phas	se			
(2×C-(H)	$_{0}(C)) + (9 \times C - (H)_{2}(C)_{2}) + (2 \times C - (H)_{2}(C)_{2})$	$(H)_2(C)(S)) +$	$\Delta_{\rm f}H^{\circ} =$	- 157.10	- 157.10	0.00	62SCO/GOO
$(1 \times S - (C)_2)$			$C_p^{\circ} =$	199.95	199.95	0.00	62SCO/GOO
` ` ` ` ` ` ` ` ` ` ` ` ` ` ` ` ` ` ` `			s° =	276.14	276.14	0.00	62SCO/GOO
	Literature - Calculated = Residua	al Reference	$\Delta_f S^\circ =$		- 568.04		
			$\Delta_t G^\circ =$		12.26		
			$\ln K_{\rm f} =$		- 4.95		
Gas phase			mari —		4.23		
•	270.37 - 269.54 - 0.83	3 69STU/WES					
$C_p^{\circ} =$	321.29 321.91 -0.62						
	727.01 727.74 -0.03	· · · · · · · · · · · · · · · · · · ·	3.Fthyl.1.n	ronene culfi	de; 4-Thia-1-h	ovono	си с
$\Delta_f S^\circ =$	-1206.93) 09310/WE3					C ₅ H ₁₀ S
					× C-(H) ₂ (C)(S		
$\Delta_{\rm f}G^{\circ} =$	90.31		(1×C-(F	$1)_{2}(C_{d})(S))$	$+(1\times C_d-(H)(0))$	J))+(1×Ca-(H)2)
$lnK_f =$	- 36.43			T itomotum	e Calculated	Bosiduol	Dafanamaa
			-	Literatur	c Calculated	- Residuai	Reference
Liquid phase							
$\Delta_{\mathbf{f}}H^{\circ} =$	-350.51		Gas phase				
$C_p^{\circ} =$	440.25		$\Delta_t H^{\circ} =$	17.80	18.27	-0.47	62MAC/MAY2
S° =	570.00						
$\Delta_{c}S^{\circ} =$	-1364.67						
$\Delta_f G^\circ =$	56.37		Liquid phas	se.			
$\ln K_{\rm f} =$	- 22.74		$\Delta_t H^\circ =$	-21.50	-24.20	2.70	62MAC/MAY2
Butyl pentad (2×C-(H) (1×S-(C) ₂	$_{3}(C)) + (15 \times C - (H)_{2}(C)_{2}) + (2 \times C$	$C_{19}H_{40}S$ -(H) ₂ (C)(S)) +		$I)_3(C))+(1$	× C-(H) ₂ (C)(S (2×-CH ₃ corr		
(2×C-(H)	$_{3}(C)) + (15 \times C - (H)_{2}(C)_{2}) + (2 \times C$	-(H) ₂ (C)(S))+	(3×C-(F	$H_{3}(C) + (1 + (1)(C)_{2}(S)) +$		r (tertiary))	C _s H ₁₂ S) ₂) + Reference
(2×C-(H) (1×S-(C) ₂	$_{3}(C)$) + $(15 \times C - (H)_{2}(C)_{2})$ + $(2 \times C)_{3}$, $\sigma = 9$	-(H) ₂ (C)(S))+	(3×C-(F (1×C-(F	$H_{3}(C) + (1 + (1)(C)_{2}(S)) +$	(2×-CH ₃ corr	r (tertiary)))2)+
(2×C-(H) (1×S-(C) ₂	$(3(C)) + (15 \times C - (H)_2(C)_2) + (2 \times C)_1$, $\sigma = 9$ Literature – Calculated = Residua	al Reference	(3×C-(F (1×C-(F	$H_{3}(C) + (1 + (1 + (1 + (1 + (1 + (1 + (1 + ($	e – Calculated	r (tertiary)) = Residual	Reference
$(2 \times C - (H))$ $(1 \times S - (C)_2$ Gas phase $\Delta_t H^\circ = -$	$(3(C)) + (15 \times C - (H)_2(C)_2) + (2 \times C)_2$ $(3(C)) + (15 \times C - (H)_2(C)_2) + (2 \times C)_2$ $(3(C)) + (15 \times C - (H)_2(C)_2) + (2 \times C)_2$ Literature – Calculated = Residual	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES	$(3 \times C - (H + (1 \times C - (H + (1 \times C - (H + (1 \times C - (H + (H$	$H_{3}(C) + (1 + (1)(C)_{2}(S)) +$	e - Calculated	r (tertiary)))2)+
$(2 \times C - (H))$ $(1 \times S - (C)_2)$ Gas phase $\Delta_t H^\circ = -C_t^\circ =$	$(3C) + (15 \times C - (H)_2(C)_2) + (2 \times C)_1$, $\sigma = 9$ Literature – Calculated = Residual Resi	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES 7 69STU/WES	(3×C-(F (1×C-(F	$H_{3}(C) + (1 + (1 + (1 + (1 + (1 + (1 + (1 + ($	e – Calculated	r (tertiary)) = Residual	Reference
$(2 \times C - (H))$ $(1 \times S - (C)_2)$ Gas phase $\Delta_t H^\circ = -C_t^\circ = S^\circ =$	$^{3}(C)$) + $(15 \times C - (H)_{2}(C)_{2})$ + $(2 \times C)$ $^{3}(C)$), $\sigma = 9$ Literature – Calculated = Residual $^{3}(C)$ = $^{3}(C)$ = $^$	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES 7 69STU/WES	$(3 \times C - (H + (1 \times C - (H + (1 \times C - (H + (1 \times C - (H + (H$	$H_{3}(C) + (1 + (1 + (1 + (1 + (1 + (1 + (1 + ($	e - Calculated	r (tertiary)) = Residual	Reference
$(2 \times C - (H))$ $(1 \times S - (C))$ Gas phase $\Delta_t H^\circ = -C_t^\circ = S^\circ = \Delta_t S^\circ =$	$^{3}(C)$) + $(15 \times C - (H)_{2}(C)_{2})$ + $(2 \times C - (H)_{2}(C)_{2})$ +	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES 7 69STU/WES	Gas phase $\Delta_t H^{\circ} = C_p^{\circ} =$	H ₃ (C)) + (1 H)(C) ₂ (S)) + Literatur - 117.20	e - Calculated	r (tertiary)) = Residual	Reference
$(2 \times C - (H))$ $(1 \times S - (C))$ Gas phase $\Delta_t H^\circ = -C_{P_t}^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	$(3C) + (15 \times C - (H)_2(C)_2) + (2 \times C)_3$, $\sigma = 9$ Literature – Calculated = Residual Resi	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES 7 69STU/WES	$(3 \times C - (H + (1 \times C - (H + (1 \times C - (H + (1 \times C - (H + (H$	H ₃ (C)) + (1 H)(C) ₂ (S)) + Literatur - 117.20	e – Calculated - 113.36 141.02	r (tertiary)) = Residual - 3.84	Reference 62MAC/MAY
$(2 \times C - (H))$ $(1 \times S - (C))$ Gas phase $\Delta_t H^\circ = -C_t^\circ = S^\circ = \Delta_t S^\circ =$	$^{3}(C)$) + $(15 \times C - (H)_{2}(C)_{2})$ + $(2 \times C - (H)_{2}(C)_{2})$ +	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES 7 69STU/WES	$(3 \times C - (H + (1 \times C - (H + (H + (1 \times C - (H + (1 \times C))))))))))))))))))))$ Liquid phas $\Delta_t H^\circ = (A_t + A_t + $	H ₃ (C)) + (1 H)(C) ₂ (S)) + Literatur - 117.20	e - Calculated - 113.36 141.02	r (tertiary)) = Residual	Reference
$(2 \times C - (H))$ $(1 \times S - (C))$ Gas phase $\Delta_t H^\circ = -C_{P_0}^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = 0$	$(3C) + (15 \times C - (H)_2(C)_2) + (2 \times C)_3$, $\sigma = 9$ Literature – Calculated = Residual Resi	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES 7 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{1}{C_p^\circ}$ Liquid phas $\Delta_t H^\circ = C_p^\circ = \frac{1}{C_p^\circ}$	H ₃ (C)) + (1 H)(C) ₂ (S)) + Literatur - 117.20	e - Calculated - 113.36 141.02 - 150.21 196.55	r (tertiary)) = Residual - 3.84	Reference 62MAC/MAY
$(2 \times C - (H))$ $(1 \times S - (C))$ Gas phase $\Delta_t H^\circ = -C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	$(3C)$) + $(15 \times C - (H)_2(C)_2)$ + $(2 \times C)$ $(3C)$), $\sigma = 9$ Literature – Calculated = Residual R	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES 7 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = $ $S^\circ = $	H ₃ (C)) + (1 H)(C) ₂ (S)) + Literatur - 117.20	- 113.36 141.02 - 150.21 196.55 304.18	r (tertiary)) = Residual - 3.84	Reference 62MAC/MAY
$(2 \times C - (H))$ $(1 \times S - (C))$ Gas phase $\Delta_t H^{\circ} = -C_{\rho}^{\circ} = S^{\circ} = \Delta_t S^{\circ} = L_{r} G^{\circ} = L_{r} G^{\circ}$	$(3C)$) + $(15 \times C - (H)_2(C)_2)$ + $(2 \times C)$ $(3C)$), $\sigma = 9$ Literature – Calculated = Residual R	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES 7 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = $ $\Delta_t G^\circ = \Delta_t G^\circ = $	H ₃ (C)) + (1 H)(C) ₂ (S)) + Literatur - 117.20	- 113.36 141.02 - 150.21 196.55 304.18 - 540.00	r (tertiary)) = Residual - 3.84	Reference 62MAC/MAY
$(2 \times C - (H))$ $(1 \times S - (C)_2)$ Gas phase $\Delta_t H^{\circ} = -C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \ln K_t = \ln K_t = -1$ Liquid phase $\Delta_t H^{\circ} = -1$	$(3C)$) + $(15 \times C - (H)_2(C)_2)$ + $(2 \times C)$ $(3C)$), $\sigma = 9$ Literature – Calculated = Residual (394.05 - 393.32 - 0.7) (458.48 + 459.25 - 0.7)	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES 7 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phas $\Delta_t H^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = $	H ₃ (C)) + (1 H)(C) ₂ (S)) + Literatur - 117.20	- 113.36 141.02 - 150.21 196.55 304.18 - 540.00 10.79	r (tertiary)) = Residual - 3.84	Reference 62MAC/MAY
Gas phase $\Delta_t H^\circ = -C_p^\circ = \Delta_t G^\circ = \ln K_t = -Liquid phase$ $\Delta_t H^\circ = -C_p^\circ = C_p^\circ = C_p^\circ = -Liquid phase$ $\Delta_t H^\circ = -C_p^\circ = C_p^\circ = -C_p^\circ = -C_p$	$^{3}(C)$) + $(15 \times C - (H)_{2}(C)_{2})$ + $(2 \times C)$ $^{3}(C)$), $\sigma = 9$ Literature – Calculated = Residual $^{3}(C)$ = $^{3}(C)$ = $^$	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES 7 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = $ $\Delta_t G^\circ = \Delta_t G^\circ = $	H ₃ (C)) + (1 H)(C) ₂ (S)) + Literatur - 117.20	- 113.36 141.02 - 150.21 196.55 304.18 - 540.00	r (tertiary)) = Residual - 3.84	Reference 62MAC/MAY
Gas phase $\Delta_t H^\circ = -C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = \Delta_t H^\circ = -C_p^\circ = S^\circ = S_t H^\circ = S^\circ $	$(3C) + (15 \times C - (H)_2(C)_2) + (2 \times C)_3$, $\sigma = 9$ Literature – Calculated = Residual Resi	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES 7 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phas $\Delta_t H^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = $	H ₃ (C)) + (1 H)(C) ₂ (S)) + Literatur - 117.20	- 113.36 141.02 - 150.21 196.55 304.18 - 540.00 10.79	r (tertiary)) = Residual - 3.84	Reference 62MAC/MAY
Gas phase $\Delta_t H^\circ = -C_p^\circ = S^\circ = \Delta_t G^\circ = \ln K_t = \Delta_t H^\circ = -C_p^\circ = S^\circ = \Delta_t H^\circ = C_p^\circ = \Delta_t H^\circ = C_p^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \frac{\Delta_t S^\circ = \Delta_t S^\circ $	$^{3}(C)$) + $(15 \times C - (H)_{2}(C)_{2})$ + $(2 \times C)$ $^{3}(C)$), $\sigma = 9$ Literature – Calculated = Residual $^{3}(C)$ = $^{3}(C)$ = $^$	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES 7 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phas $\Delta_t H^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = $	H ₃ (C)) + (1 H)(C) ₂ (S)) + Literatur - 117.20	- 113.36 141.02 - 150.21 196.55 304.18 - 540.00 10.79	r (tertiary)) = Residual - 3.84	Reference 62MAC/MAY
Gas phase $\Delta_t H^{\circ} = -C_p^{\circ} = S^{\circ} = \Delta_t G^{\circ} = InK_t = InK_t = C_p^{\circ} = S^{\circ} = S^{\circ}$	$(3C) + (15 \times C - (H)_2(C)_2) + (2 \times C)_3$, $\sigma = 9$ Literature – Calculated = Residual Resi	-(H) ₂ (C)(S)) + al Reference 3 69STU/WES 7 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phas $\Delta_t H^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = $	H ₃ (C)) + (1 H)(C) ₂ (S)) + Literatur - 117.20	- 113.36 141.02 - 150.21 196.55 304.18 - 540.00 10.79	r (tertiary)) = Residual - 3.84	Reference 62MAC/MAY

TABLE 43. Sulfides (32) - Continued

(4×C-(H		× C-(H)2(C)(S) ×-CH3 corr (qu		C ₆ H ₁₄ () ₂) +
····	Literature	e – Calculated	= Residual	Reference
Gas phase				
	- 148.00	- 145.38	-2.62	62MAC/MAY
C _p =		163.48		100 to
Liquid phas	se			
	- 187.30	183.87	-3.43	62MAC/MAY
$C_p^{\circ} =$		224.13		
S° =		317.23		
$\Delta_{\mathbf{f}}S^{\circ} =$		- 663.26		
$\Delta_f G^\circ =$		13.88		
$lnK_f =$		-5.60		
(3×C-(I				C_7H_{14} or (quaternary)) + $(1 \times C_d - (H)(C)$
	Literatur	e – Calculated	= Residual	Reference
Gas phase Δ _t H° =	-46.70	-43.24	-3.46	62MAC/MAY
Liquid pha Δ _t H° =		-89.13	-1.87	62MAC/MAY
Diphenyl so (2×C _B -(C _B ~(H)(C _B) ₂)+	$(1 \times S - (C_B)_2)$	C ₁₂ H ₁₀ :
	Literatur	e – Calculated	= Residual	Reference
Gas phase				
$\Delta_t H^\circ =$	231.20	231.20	0.00	62MAC/MAY
$C_p^{\circ} =$		187.86		
Liquid pha				
$\Delta_t H^\circ =$	163.40	163.40	0.00	62MAC/MAY
C _p =	271.12	271.12	0.00	31SMI/AND2
	nyl sulfide H)3(S))+(1>	< S-(C _B)(C))+	(1 × C _B -(S)) +	С ₇ H ₈ ! - (5 × С _в (H)(С _в) ₂

Gas phase $\Delta_t H^\circ =$

97.30

98.25

-0.95

72GOO2

	Literatur	e – Calculated	= Residual	Reference
Liquid pha	ise			
$\Delta_t H^\circ =$	43.00	45.78	-2.78	72GOO2
$C_p^{\circ} =$	206.02	206.02	0.00	74MES/FIN
s° =	252.50	252.50	0.00	74MES/FIN
$\Delta_{\mathbf{f}}S^{\circ} =$		-342.02		
$\Delta_{\mathbf{f}}G^{\circ} =$		147.75		
$lnK_f =$		-59.60		
(1×C-(H) ₃ (C))+(1 (S))+(5×C ₁	. , , , -,-,		
	H) ₃ (C))+(1 (S))+(5×C ₁			
(1×C-(H) ₃ (C))+(1 (S))+(5×C ₁	$_{B}$ -(H)(C _B) ₂)		3)(C))+
(1×C-(1 (1×C _B -	H) ₃ (C))+(1 (S))+(5×C ₁	$_{B}$ -(H)(C _B) ₂)		Reference
$(1 \times C - (1 \times C_B - 1 \times $	H) ₃ (C)) + (1 (S)) + (5 × C ₁ Literatur 77.00	e — Calculated	- Residual	Reference
(1×C-(1 (1×C _B -	H) ₃ (C)) + (1 (S)) + (5 × C ₁ Literatur 77.00	g-(H)(C _B) ₂) e Calculated	- Residual	Reference
$(1 \times C - (1 \times C_B - 1 \times $	H) ₃ (C)) + (1 (S)) + (5 × C ₁ Literatur 77.00	75.08	Residual	Reference
$(1 \times C_{-}(1 \times C_{B} - 1 \times C$	H) ₃ (C)) + (1 (S)) + (5 × C ₁ Literatur 77.00	75.08	Residual	Reference
$(1 \times C - (1 \times C_B - 1 \times $	H) ₃ (C)) + (1 (S)) + (5 × C ₁ Literatur 77.00	75.08 19.01 230.20	Residual	Reference
$(1 \times C - (1 \times C_B - 1 \times $	H) ₃ (C)) + (1 (S)) + (5 × C ₁ Literatur 77.00	75.08 19.01 230.20 293.59	Residual	3)(C))+

TABLE 44. Disulfides (8)

TABLE 44. Disulfides (8) - Continued

Dimethyl di (2×C-(H		×S-(C)(S)), σ	$C)(S)), \sigma = 18$		Dipropyl disulfide (Continued) $(2 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)_2) + (2 \times C - (H)_$				$C_{\epsilon}H_{1\epsilon}S_{\epsilon}$ $O_{2}(C)(S)) +$	
	Literatur	e – Calculated	= Decidual	Reference	(2×S-($C)(S)), \sigma =$	18			
	Literatur					Literatu	re – Calculated	= Residual	Reference	
Gas Phase										
$\Delta_t H^\circ = $	-24.41	-29.28	4.87	58HUB/DOU	Liquid Ph	ase				
$C_p^{\circ} =$	94.31	97.96	-3.65	69STU/WES	$\Delta_{\rm f}H^{\circ} =$	-171.50	- 171.50	0.00	58HUB/DOU	
S° =	336.64	331.61	5.03	69STU/WES	$C_p^{\circ} =$	262.46	263.58	-1.12	58HUB/DOU	
$\Delta_f S^\circ =$		- 135.69			<i>S</i> ° =	373.55	375.22	- 1.67	58HUB/DOU	
$\Delta_{\rm f}G^{\circ} =$		11.18			$\Delta_i S^\circ =$		-637.33			
$lnK_f =$		-4.51			$\Delta_t G^{\circ} =$		18,52			
					$lnK_f =$		-7.47			
Liquid Pha	se									
$\Delta_t H^\circ =$	-62.60	-66.50	3.90	58HUB/DOU						
$C_n^{\circ} =$	146.11	154.38	-8.27	50SCO/FIN	Dibutyl dis	sulfide			C ₈ H ₁₈ S	
S° =	235.29	228.28	7.01	50SCO/FIN	(2×C-($H_{3}(C)) + (4$	$\times C-(H)_2(C)_2$	$+(2\times C-(H)_{2})$		
$\Delta_f S^{\circ} =$		-239.02				$C)(S)), \sigma =$		(3-1-)2	(-)(-))	
$\Delta_{\mathbf{f}}G^{\circ} =$		4.76			((-)(-)), -				
$\ln K_{\rm f} =$		-1.92				Literatu	re – Calculated	= Residual	Reference	
					Gas Phase					
Diethyl dis	ulfida			C4H10S2	$\Delta_t H^\circ =$	- 158.41	- 158.14	-0.27	64MAC/MCC	
		~ C (II) (C)(S))		-	231.08	231.32		,	
(2 X C-(1	1)3(C))+(2	\times C-(H) ₂ (C)(S))+(2×3-(C	$J(S)J, \sigma = 10$	$C_p^{\circ} =$			-0.24	69STU/WES	
			D -11 -1	Defe	S° =	572.83	571.99	0.84	69STU/WES	
	Literatu	re – Calculated	= Residual	Reference	$\Delta_{f}S^{\circ} =$		-713.18			
					$\Delta_{\mathbf{f}}G^{\circ} =$		54.49			
Gas Phase					$lnK_f =$		-21.98			
$\Delta_i H^\circ =$	-74.64	- 75.62	0.98	58HUB/DOU						
$C_{\rho}^{\circ} =$	141.34	139.76	1.58	69STU/WES	Liquid Pha	ase				
S° =	414.51	415.35	-0.84	69STU/WES	$\Delta_t H^\circ =$	- 222.90	- 222.96	0.06	64MAC/MCC	
Δ _f S° –	111.01	- 324.58	0.0 .	0,010,1120	$C_p^{\alpha} =$	222.70	324,42	0.00	0 11111 10/11100	
$\Delta_t G^{\circ} =$		21.15			S° =		439.98			
$lnK_f =$		-8.53			$\Delta_{f}S^{\circ} =$		-845.19			
umzi		- 0.55			$\Delta_i G^\circ =$		29.03			
					$\ln K_{\rm f} =$		-11.71			
Liquid Pha AH° =		- 120.04	-0.06	58HUB/DOU					.,	
	-120.10									
$C_p^{\circ} = S^{\circ} =$	204.01	202.74	1.27	52SCO/FIN	D!4-1-1				~ ** C	
	305.01	310.46	-5.45	52SCO/FIN	Dipentyl d			. (00 (77)	C ₁₀ H ₂₂ S	
$\Delta_f S^\circ =$		-429.46					$6 \times C - (H)_2(C)_2$	+ (2 × C−(H) ₂ ((C)(S))+	
$\Delta_{\rm f}G^{\circ} =$		8.00			(2×S-(0	$C)(S)), \sigma =$	18			
$\ln K_f =$		- 3.23				Literatu	re – Calculated	= Residual	Reference	
					- Carren					
Dipropyl d		2×C-(H) ₂ (C) ₂)	+ (2 × C-(H) ₂	$C_6H_{14}S_2$ (C)(S)) +	Gas Phase $\Delta_t H^* =$	- 199.62	199.40	-0.22	69STU/WES	
	$C)(S)), \sigma =$		(= -72	V - 7 V - 7 / -	$C_p^{\circ} =$	276.81	277.10	-0.29	69STU/WES	
(= u (-/(-//, -				S° =	650.74	650.31	0.43	69STU/WES	
	Literatu	re – Calculated	= Residual	Reference	$\Delta_{r}S^{\circ} =$	000117	- 907.48	J.1J	0,0 L O/ 11 LO	
	Literatu	Carculated	1.00,000		$\Delta_f G^\circ =$		71.17			
					$\ln K_{\rm f} =$		-28.71			
Gas Phase $\Delta_t H^\circ =$		_ 116 99	_0.21	SSHITE/DOTT						
	-117.19	-116.88	-0.31	58HUB/DOU	Liquid DL	200				
$C_p^{\circ} =$	185.35	185.54	-0.19	69STU/WES	Liquid Pha	180	074.40			
S° =	494.97	493.67	1.30	69STU/WES	$\Delta_{\rm f}H^{\circ} =$		-274.42			
$\Delta_f S^\circ =$		-518.88			$C_p^{\circ} =$		385.26			
$\Delta_{\rm f}G^{\circ} =$		37.82			<i>S</i> ° =		504.74			
$lnK_f =$		- 15.26			$\Delta_f S^\circ =$		- 1053.05			
					$\Delta_{\rm f}G^{\circ} =$		39.55			
					$lnK_f =$		-15.95			

TABLE 44.	Disulfides	(8) $-$	Continued
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TABLE 45. Sulfoxides (6)

Dihexyl disulfide $(2 \times C - (H)_3(C)) + (8 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(C)_2)$ $(2 \times 2 + (C)(S)) = 18$	(S))+	Dimethyl so (2×C-(H		(1×SO-(C) ₂), o	$\sigma = 18$	C ₂ H ₆ Os
$(2 \times S-(C)(S))$, $\sigma = 18$ Literature – Calculated = Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas Phase $\Delta_t H^\circ = -240.83 - 240.66 -0.17$ $C_p^\circ = 322.54 322.88 -0.34$ $S^\circ = 728.64 728.63 0.01$ $\Delta_t S^\circ = -1101.78$ $\Delta_t G^\circ = 87.84$ $\ln K_t = -35.43$	69STU/WES 69STU/WES 69STU/WES	Gas phase $ \Delta_t H^\circ = C_p^\circ - S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	-151.30 88.95 306.27	- 151.30 88.61 306.34 - 231.43 - 82.30 33.20	0.00 0.34 - 0.07	48DOU 62MAC/OHA 62MAC/OHA
Liquid Phase $ \Delta_t H^\circ = -325.88 $ $ C_\rho^\circ = 446.10 $ $ S^\circ = 569.50 $ $ \Delta_t S^\circ = -1260.91 $ $ \Delta_t G^\circ = 50.06 $ $ \ln K_t = -20.19 $		Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	se - 204.20 153.18 188.78	- 204.20 153.18 188.78 - 348.99 - 100.15 40.40	0.00 0.00 0.00	46DOU 70CLE/WES 70CLE/WES
Didecyl disulfide $(2 \times C - (H)_3(C)) + (16 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(C)_2) + (2$	C ₂₀ H ₄₂ S ₂	Diethyl sul (2×C-(F	(C) + (2	× C-(H)2(C)(S		C ₄ H ₁₀ OS -(C) ₂) Reference
Literature – Calculated = Residual	Reference	Gas phase $\Delta_t H^{\circ} =$	-205.60	- 209.62	4.02	61MAC/OHA4
Gas Phase $ \Delta_t H^\circ = -405.72 -405.70 -0.02 $ $ C_p^\circ = 505.51 506.00 -0.49 $ $ S^\circ = 1040.23 1041.91 -1.68 $ $ \Delta_t S^\circ = -1878.99 $ $ \Delta_t G^\circ = 154.52 $	69STU/WES 69STU/WES 69STU/WES	Liquid phas Δ _t H° -	se 268.00	277.96	9.96	61MAC/OIIA4
$lnK_f = -62.33$ Liquid Phase $\Delta_t H^o = -531.72$ $C_p^o = 689.46$	·		$(1)_3(C) + (1)_3(C_d)(SO)$	\times C-(H) ₂ (C)(S 1) + (1 \times C _d -(H) re – Calculated:	(C)) + $(1 \times C_{d}$	
$S^{\circ} = 828.54$ $\Delta_t S^{\circ} = -2092.36$ $\Delta_t G^{\circ} = 92.12$ $\ln K_t = -37.16$		Gas phase $\Delta_t H^\circ =$	-103.70	- 103.12	- 0.58	61MAC/OHA4
Diphenyl disulfide $(10 \times C_B - (H)(C_B)_2) + (2 \times C_B - (S)) + (2 \times S - (C_B)(S))$	C ₁₂ II ₁₀ S ₂	Liquid phas ΔμΙ° –	se -173.30	- 173.30	0.00	61MAC/OHA4
Literature - Calculated = Residual	Reference	Dipropyl su				C6H14OS
Gas Phase $\Delta_t H^\circ = 243.50$ 243.50 0.00	62MAC/MAY2	(2×C-(F (1×SO-	(C) ₂)	\times C-(H) ₂ (C) ₂) - $e - Calculated = Calculated$		C)(SO))+ Reference
Solid Phase $\Delta_t H^{\circ} = 148.50$ 148.50 0.00	62MAC/MAY2	Gas phase $\Delta_l H^\circ =$	- 254.90	- 250.88	-4.02	61MAC/OHA4

TABLE 46. Sulfones (38)

TABLE 45.	Sulfoxides	(6) —	Continued
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		< C-(H) ₂ (C) ₂) +	(2×C-(H) ₂	C ₆ H ₁₄ OS (C)(SO))+	Dimethyl so (2×C-(I		$(1 \times SO_2 - (C)_2),$	$\sigma = 18$	C ₂ H ₆ O ₂ S
(1/30/(e – Calculated =	Residual	Reference		Literatu	re – Calculated =	= Residual	Reference
					Gas phase				
Liquid phase	e				$\Delta_f H^\circ =$	-373.10	-373.10	0.00	70MAC/STE
	- 329.40	-329.42	0.02	61MAC/OHA4	$C_p^{\circ} =$	100.00	100.00	0.00	62MAC/OHA
<u> </u>					s° =	317.98	317.98	0.00	62MAC/OHA
					$\Delta_{\mathbf{f}}S^{\circ} =$		-322.31		
					$\Delta_{\mathbf{f}}G^{\circ} =$		-277.00		
ert-Butyl et	hyl sulfoxid	le		C ₆ H ₁₄ OS	$lnK_f =$		111.74		
(4×C-(H	$()_3(C)) + (1)$	\times C-(H) ₂ (C)(SC	D))+(1×SO-	-(C) ₂) +					
		3×-CH ₃ corr (c		· /-/					
	,-	- `	• • • • • • • • • • • • • • • • • • • •		Liquid pha	se			
	Literatur	e – Calculated =	Residual	Reference	$\Delta_t H^\circ =$		-436.36	0.00	
Gas phase					Solid phase	•			
$\Delta_{\mathbf{f}}H^{\circ} =$	- 274.10	-274.10	0.00	61MAC/OHA4	$\Delta_{\rm f}H^{\circ} =$	-450.10	-450.10	0.00	61BUS/MAC
					$C_p^{\circ} =$	125.35	125.35	0.00	70CLE/WES
					S° =	145.48	145.48	0.00	70CLE/WES
Liquid phas	e				$\Delta_f S^\circ =$		- 494.81		
$\Delta_t H^\circ = -$		-348.50	0.00	61MAC/OHA4	$\Delta_{\rm f}G^{\circ} =$		-302.57		
		- 1-1-			$\ln K_{\rm f} =$		122.06		
		-(2×C _B -(SO))	+(1×SO-(C	C ₁₂ H ₁₀ OS	Ethyl meth		~C.(H) (SO.))) + (1 × C (H)	
	(H)(C _B) ₂)+	- (2×C _B -(SO)) - e – Calculated =	,			$H_{3}(C)+(1$	× C-(H) ₃ (SO ₂)))+(1×C-(H)	
Diphenyl su (10×C _B -	(H)(C _B) ₂)+		,	(B) ₂)	(1×C-(I	$(C)_{3} + (1)_{3} + (1)_{3} + (1)_{2}$	\times C-(H) ₃ (SO ₂)) re Calculated =		$C_3H_8O_2S_2(C)(SO_2)) +$ Reference
(10 × C _B −	(H)(C _B) ₂)+		,	(B) ₂)	(1×C-(I (1×SO ₂ -	$(C)_{3} + (1)_{3} + (1)_{3} + (1)_{2}$			$_{2}(C)(SO_{2})) +$
(10×C _B -	(H)(C _B) ₂) + Literatur	e – Calculated =	= Residual	Reference	(1×C-(I (1×SO ₂ -	H) ₃ (C))+(1 -(C) ₂) Literatur	re Calculated =	= Residual	Reference
(10×C _B -	(H)(C _B) ₂) + Literatur	e – Calculated =	= Residual	Reference	(1×C-(I (1×SO ₂ -	$(C)_{3} + (1)_{3} + (1)_{3} + (1)_{2}$			$_{2}(C)(SO_{2})) +$
(10×C _B -	(H)(C _B) ₂) + Literatur	e – Calculated =	= Residual	Reference	$(1 \times C - (1 \times SO_2)^2)$ $(1 \times SO_2)^2$ $Gas phase$ $\Delta_t H^\circ =$	H ₃ (C)) + (1 -(C) ₂) Literatur - 408.36	re Calculated =	= Residual	Reference
(10×C _B -	(H)(C _B) ₂) + Literatur	e – Calculated =	= Residual	Reference	$(1 \times C - (I \times SO_2)^2)$ $Gas phase$ $\Delta_t H^\circ =$ $Liquid phase$	H ₃ (C)) + (1 -(C) ₂) Literatur - 408.36	- 400.13	= Residual	Reference
(10×C _B -	(H)(C _B) ₂) + Literatur	e – Calculated =	= Residual	Reference	$(1 \times C - (1 \times SO_2)^2)$ $(1 \times SO_2)^2$ $Gas phase$ $\Delta_t H^\circ =$	H ₃ (C)) + (1 -(C) ₂) Literatur - 408.36	re Calculated =	= Residual	Reference
(10×C _B -	(H)(C _B) ₂) + Literatur	e – Calculated =	= Residual	Reference	$(1 \times C - (I \times SO_2)^2)$ $Gas phase$ $\Delta_t H^\circ =$ $Liquid phase$	H ₃ (C)) + (1 -(C) ₂) Literatur - 408.36	- 400.13	= Residual	Reference
(10×C _B -	(H)(C _B) ₂) + Literatur	e – Calculated =	= Residual	Reference	$(1 \times C - (I \times SO_2)^2)$ $Gas phase$ $\Delta_t H^\circ =$ $Liquid phase$	H ₃ (C)) + (1 -(C) ₂) Literatur - 408.36	- 400.13	= Residual	Reference
(10×C _B -	(H)(C _B) ₂) + Literatur	e – Calculated =	= Residual	Reference	$(1 \times C - (H + C + C))^{-1}$ Gas phase $\Delta_t H^{\circ} =$ Liquid phase $\Delta_t H^{\circ} =$	H ₃ (C)) + (1 -(C) ₂) Literatur - 408.36	- 400.13	= Residual	Reference
(10×C _B -	(H)(C _B) ₂) + Literatur	e – Calculated =	= Residual	Reference	$(1 \times C - (1 \times SO_2)^2)$ Gas phase $\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ Solid phase	H ₃ (C)) + (1 -(C) ₂) Literatur - 408.36	- 400.13 - 470.12	= Residual - 8.23	Reference 70MAC/STE
(10×C _B -	(H)(C _B) ₂) + Literatur	e – Calculated =	= Residual	Reference	$(1 \times C - (1 \times SO_2)^2)$ Gas phase $\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$ Solid phase	H ₃ (C)) + (1 -(C) ₂) Literatur - 408.36	- 400.13 - 470.12	= Residual - 8.23	Reference 70MAC/STE
(10×C _B -	(H)(C _B) ₂) + Literatur	e – Calculated =	= Residual	Reference	$(1 \times C - (H + C + C))^{-1}$ Gas phase $\Delta_t H^\circ = $	H ₃ (C)) + (1 -(C) ₂) Literatur - 408.36 se - 486.06	- 400.13 - 470.12	- 8.23 0.00	Reference 70MAC/STE 61BUS/MAC
(10×C _B -	(H)(C _B) ₂) + Literatur	e – Calculated =	= Residual	Reference	$(1 \times C - (H + C + C))^{-1}$ Gas phase $\Delta_t H^\circ = $	$H_{3}(C) + (1 - (C)_{2})$ Literatus -408.36 se -486.06 fone $H_{12} + (2 \times 6)$	- 400.13 - 470.12 - 486.06	-8.23 0.00 (1 × SO ₂ -(C _d	Reference 70MAC/STE 61BUS/MAC

 $\Delta_t H^{\circ} = -150.90$

- 150.90

0.00

69MAC/MCN

Allyl methyl sulfone $(1 \times C_{d}-(H)_2) + (1 \times C_{d}-(H)(C)) + (1 \times C_{-}(H)_2(C_d)(S_{-}(1 \times SO_2-(C)_2) + (1 \times C_{-}(H)_3(SO_2))$	C ₄ H ₈ O ₂ S SO ₂))+	Butyl methyl sulfone $C_5H_{12}O_2S$ $(1 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)(SO_2)) + (1 \times SO_2 - (C)_2) + (1 \times C - (H)_3(SO_2))$
Literature – Calculated = Residual	Reference	Literature – Calculated = Residual Reference
Gas phase $\Delta_t H^\circ = -305.60 -297.69 -7.91$	70MAC/STE	Gas phase $\Delta_t H^{\circ} = -459.40 -441.39 -18.01$ 70MAC/STE
Liquid phase $\Delta_t H^\circ = -384.70 -385.00 0.30$	70MAC/STE	Liquid phase $\Delta_t H^\circ = -535.55 -521.58 -13.97$ 61MAC/OHA
Diethyl sulfone $(2 \times C-(H)_3(C)) + (2 \times C-(H)_2(C)(SO_2)) + (1 \times SO_2)$		tert-Butyl methyl sulfone $(1 \times C - (H)_3(SO_2)) + (1 \times SO_2 - (C)_2) + (1 \times C - (C)_3(SO_2)) + (3 \times C - (H)_3(C)) + (3 \times - CH_3 \text{ corr (quaternary))}$
Literature – Calculated = Residual	Reference	Literature - Calculated = Residual Reference
Gas phase $\Delta_t H^{\circ} = -428.86 -427.16 -1.70$	70MAC/STE	Gas phase $\Delta_t H^\circ = -473.20 - 469.78 - 3.42$ 70MAC/STE
Liquid phase $\Delta_t H^\circ = -503.88$		Solid phase $\Delta_t H^\circ = -555.68 -552.85 -2.83$ 61BUS/MAC
Solid phase $\Delta_t H^\circ = -515.20 -522.02$ 6.82	61MAC/OHA	tert-Butyl ethyl sulfone $C_4H_{14}O_2S$ $(4\times C-(H)_3(C))+(1\times C-(H)_2(C)(SO_2))+(1\times SO_2-(C)_2)+$
Isopropyl methyl sulfone $(1 \times C - (H)_3(SO_2)) + (1 \times SO_2 - (C)_2) + (1 \times C - (H)(C)_2 + (2 \times -CH_3) + (2 \times C - (H)_3(C))$	$C_4H_{10}O_2S$ $O_2(SO_2)) +$	$(1 \times C - (C)_3(SO_2)) + (3 \times -CH_3 \text{ corr (quaternary)})$ $\text{Literature - Calculated = Residual} \qquad \text{Reference}$
Literature - Calculated = Residual	Reference	Gas phase $\Delta_i H^\circ = -491.40 -496.81$ 5.41 61MAC/OHA
Gas phase $\Delta_t H^\circ = -434.00 -433.88 -0.12$	61BUS/MAC	Liquid phase $\Delta_t H^{\circ} = -578.00 -578.51$ 0.51 61MAC/OHA
Allyl ethyl sulfone $ (1 \times C_{d^{-}}(H)_2) + (1 \times C_{d^{-}}(H)(C)) + (1 \times C - (H)_2(C_d)(S_{d^{-}}(1 \times SO_2 - (C)_2) + (1 \times C - (H)_2(C)(SO_2)) + (1 \times C - $		Di-tert-butyl sulfone $(6 \times C - (H)_3(C)) + (1 \times SO_2 - (C)_2) + (2 \times C - (C)_3(SO_2)) + (6 \times -CH_3 \text{ corr } (quat/quat))$
		Literature – Calculated = Residual Reference
Gas phase $\Delta_1 H^\circ = -322.17 - 324.72$ 2.55	70MAC/STE	Gas phase $\Delta_t H^\circ = -546.00 - 542.94 - 3.06$ 70MAC/STE
Liquid phase $\Delta_t H^\circ = -405.64 -418.76$ 13.12	61MAC/OHA	Solid phase $\Delta_t H^{\circ} = -640.07 - 642.94$ 2.87 61MAC/OHA

Dipropyl sulfone $(2 \times C-(H)_3(C)) + (2 \times C-(H)_2(C)_2) + (2 \times C-(H)_2(C)_2) + (2 \times C-(H)_2(C)_2)$ $(1 \times SO_2-(C)_2)$	$C_6H_{14}O_2S$ $S(SO_2)$ +		$H)_2)+(1\times$	C_d -(H)(SO ₂)) + + (5 × C_B -(H)($C_8H_8O_2S$ $(C_B)) +$
Literature – Calculated = Residual	Reference		Literatu	e – Calculated	= Residual	Reference
Gas phase $\Delta_0 H^{\circ} = -467.77 - 468.42 = 0.65$	70MAC/STE	Gas phase Δ ₁ II° -	- 129.00	- 129.12	0.12	69MAC/MCN
Liquid phase $\Delta_t H^\circ = -547.85 - 555.34$ 7.49	61MAC/OHA		(C) + (1)	× C _B -(C)(C _B) ₂) + (1 × SO ₂ -(C)		
Dibutyl sulfone (2 × C-(H) ₃ (C)) + (4 × C-(H) ₂ (C) ₂) + (2 × C-(H) ₂ (C) (1 × SO ₂ -(C) ₂)	C ₈ H ₁₈ O ₂ S)(SO ₂)) +		Literatur	e – Calculated	= Residual	Reference
Literature – Calculated = Residual	Reference	Gas phase $\Delta_t H^\circ =$	- 273.10	- 279.26	6.16	61МАС/ОНА
Gas phase $\Delta_t H^\circ = -509.60 -509.68$ 0.08	70MAC/STE		H)3(SO2))+	(1×SO ₂ -(C) ₂) (5×C _B -(H)(C _B		C ₈ H ₁₉ O ₂ ; (C _B)(SO ₂)) +
Liquid phase $\Delta_t H^\circ = -606.80$		(1×08 (e – Calculated		Reference
Solid phase $\Delta_t H^\circ = -609.86 - 639.66$ 29.80	61BUS/MAC	Gas phase Δ _t H° =	- 272.10	- 267.95	- 4.15	61BUS/MAC
Diisobutyl sulfone $(4 \times C-(H)_3(C)) + (2 \times C-(H)(C)_3) + (4 \times -CH_3 \text{ corr}$ $(2 \times C-(H)_2(C)(SO_2)) + (1 \times SO_2-(C)_2)$	C ₈ H ₁₈ O ₂ S (tertiary))+		$I_{3}(C) + (1$	nzene × C ₁ -(C)) + (1 × (1 × C _B -(SO ₂)(C ₉ H ₈ O ₂ S _B –(H)(C _B) ₂)
Literature - Calculated = Residual	Reference	· .	Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^{\circ} = -535.15 -523.06 -12.09$	70MAC/STE	Gas phase $\Delta_t H^\circ =$	43.20	38.17	5.03	69MAC/STE3
Liquid phase $\Delta_t H^\circ = -624.84 - 617.36 - 7.48$	61МАС/ОНА	, ,	H))+(1×C	nzene ,-(C)) + (1 × C- (1 × C _B -(SO ₂)(· /-· // -	,,
Methyl phenyl sulfone $(1 \times C - (H)_3(SO_2)) + (1 \times SO_2 - (C)(C_B)) + (1 \times C_B - (S)(C_B))$	$C_7H_8O_2S$ $O_2)(C_B)_2) +$			e – Calculated =		Reference
$(5 \times C_B - (H)(C_B)_2)$ Literature - Calculated = Residual	Reference	Gas phase $\Delta_t H^\circ =$	36.20	40.39	-4.19	69MAC/STE3
Gas phase $\Delta_t H^{\circ} = -253.40 -246.83 -6.57$	61MAC/OHA2					

Allenyl phenyl sulfone $C_9H_8O_2S$ $(1 \times C_d-(H)_2) + (1 \times C_a) + (1 \times C_d-(H)(SO_2)) +$ $(1 \times SO_2-(C_d)(C_B)) + (1 \times C_B-(SO_2)(C_B)_2) + (5 \times C_B-(H)(C_B)_2)$ Literature – Calculated = Residual Reference	$ \begin{array}{ll} \textbf{(E)-1-Methyl-4-(1-propenylsulfonyl)benzene} & \textbf{C_{10}H$_{12}$O}_2$S\\ \textbf{(1}\times C-(H)_3(C)) + \textbf{(1}\times C_B-(C)(C_B)_2) + \textbf{(4}\times C_B-(H)(C_B)_2) + \\ \textbf{(1}\times C_B-(SO_2)(C_B)_2) + \textbf{(1}\times SO_2-(C_d)(C_B)) + \textbf{(1}\times C_d-(H)(SO_2)) + \\ \textbf{(1}\times C_d-(H)(C)) + \textbf{(1}\times C-(H)_3(C)) \end{array} $
Literature - Calculated - Residual Reference	Literature – Calculated = Residual Reference
Gas phase $\Delta_t H^{\circ} = 1.80$ 13.55 -11.75 70MAC/STE	Gas phase $\Delta_t H^\circ = -208.90 -193.81 -15.09$ 69MAC/MCN
$ \begin{array}{c} \text{p-Tolyl vinyl sulfone} & C_9H_{10}O_2S \\ (1\times C-(H)_3(C)) + (1\times C_B-(C)(C_B)_2) + (4\times C_B-(H)(C_B)_2) + \\ (1\times C_B-(SO_2)(C_B)_2) + (1\times SO_2-(C_d)(C_B)) + (1\times C_d-(H)(SO_2)) + \\ (1\times C_d-(H)_2) & \\ \\ \text{Literature} - \text{Calculated} = \text{Residual} & \text{Reference} \end{array} $	$ \begin{array}{ll} \mbox{1-Methyl-4-(2-propenylsulfonyl)benzene} & C_{10}H_{12}O_2S \\ (1\times C-(H)_3(C)) + (1\times C_B-(C)(C_B)_2) + (4\times C_B-(H)(C_B)_2) + \\ (1\times C_B-(SO_2)(C_B)_2) + (1\times SO_2-(C)(C_B)) + (1\times C-(H)_2(C_d)(SO_2)) + \\ (1\times C_d-(H)(C)) + (1\times C_d-(H)_2) \\ \\ \mbox{Literature} - Calculated = Residual & Reference \\ \end{array} $
Gas phase $\Delta_t H^{\circ} = -162.30 - 161.55 - 0.75$ 69MAC/MCN	Gas phase $\Delta_t H^{\circ} = -203.30 -203.85$ 0.55 69MAC/MCN
$ \begin{array}{ll} \mbox{1-Methyl-4-(1-propynylsulfonyl)benzene} & C_{10}H_{10}O_2S \\ (1\times C-(H)_3(C)) + (1\times C_B-(C)(C_B)_2) + (4\times C_B-(H)(C_B)_2) + \\ (1\times C_B-(SO_2)(C_B)_2) + (1\times SO_2-(C_1)(C_B)) + (1\times C_t-(SO_2)) + \\ (1\times C_t-(C)) + (1\times C-(H)_3(C)) \\ \\ \mbox{Literature} - Calculated = Residual & Reference \\ \end{array} $	$ \begin{array}{ll} \hbox{\bf 1-Methyl-4-(1-methylethenylsulfonyl)benzene} & C_{10}H_{12}O_2S\\ (1\times C-(H)_3(C))+(1\times C_B-(C)(C_B)_2)+(4\times C_B-(H)(C_B)_2)+\\ (1\times C_B-(SO_2)(C_B)_2)+(1\times SO_2-(C_d)(C_B))+(1\times C_d-(C)(SO_2))+\\ (1\times C_d-(H)_2)+(1\times C-(H)_3(C))\\ \\ \hbox{Literature-Calculated=Residual} & Reference \\ \end{array} $
Gas phase $\Delta_t H^\circ = 10.10$ 5.74 4.36 69MAC/STE3	Gas phase $\Delta_i H^o = -196.70 -191.38 -5.32$ 69MAC/MCN
$ \begin{array}{ll} \mbox{1-Methyl-4-(2-propynylsulfonyl)benzene} & C_{10}H_{10}O_2S \\ (1\times C-(H)_3(C)) + (1\times C_{B^-}(C)(C_B)_2) + (4\times C_{B^-}(H)(C_B)_2) + \\ (1\times C_{B^-}(SO_2)(C_B)_2) + (1\times SO_2-(C)(C_B)) + (1\times C-(H)_2(C_i)(SO_2)) + \\ (1\times C_{r^-}(C)) + (1\times C_{r^-}(H)) \\ \\ \mbox{Literature} - Calculated = Residual & Reference \\ \end{array} $	$ \begin{array}{ll} \text{1-Methyl-4-(3-butenylsulfonyl)benzene} & C_{11}H_{14}O_2S\\ (1\times C-(H)_3(C)) + (1\times C_{B^-}(C)(C_B)_2) + (4\times C_{B^-}(II)(C_B)_2) + \\ (1\times C_{B^-}(SO_2)(C_B)_2) + (1\times SO_2-(C)(C_B)) + (1\times C-(H)_2(C)(SO_2)) + \\ (1\times C-(H)_2(C)(C_d)) + (1\times C_{d^-}(H)(C)) + (1\times C_{d^-}(H)_2) \\ \\ \text{Literature} - \text{Calculated} = \text{Residual} & \text{Reference} \end{array} $
Gas phase $\Delta_t H^{\circ} = 0.70$ 7.96 -7.26 69MAC/STE3	Gas phase $\Delta_t H^{\circ} = -226.00 -222.27 -3.73$ 69MAC/MCN
$ \begin{array}{ll} \hbox{\bf 1-Methyl-4-(1,2-propadienylsulfonyl)benzene} & C_{10}H_{10}O_2S \\ \hbox{\bf (1\times C-(H)_3(C))+(1\times C_{B^-}(C)(C_B)_2)+(4\times C_{B^-}(H)(C_D)_2)+} \\ \hbox{\bf (1\times C_{B^-}(SO_2)(C_B)_2)+(1\times SO_2-(C_d)(C_B))+(1\times C_d-(H)(SO_2))+} \\ \hbox{\bf (1\times C_a)+(1\times C_{d^-}(H)_2)} \\ \\ \hbox{\bf Literature-Calculated=Residual} & \hbox{\bf Reference} \\ \end{array} $	$ \begin{array}{ll} \mbox{1-Methyl-4-(2-butenylsulfonyl)benzene} & C_{11}H_{14}O_2S \\ (1\times C-(H)_3(C)) + (1\times C_B-(C)(C_B)_2) + (4\times C_B-(H)(C_B)_2) + \\ (1\times C_B-(SO_2)(C_B)_2) + (1\times SO_2-(C)(C_B)) + (1\times C-(H)_2(C_d)(SO_2)) + \\ (2\times C_d-(H)(C)) + (1\times C-(H)_3(C)) \\ \\ \mbox{Literature} - \mbox{Calculated} = \mbox{Residual} & \mbox{Reference} \end{array} $
Gas phase $\Delta_t H^\circ = -32.60 - 18.88 - 13.72$ 69MAC/STE3	Gas phase $\Delta_t H^{\circ} = -240.80 -236.11 -4.69$ 69MAC/MCN

$ \begin{array}{l} \textbf{1-Methyl-4-(1-butenylsulfonyl)benzene} \\ (1 \times C-(H)_3(C)) + (1 \times C_B-(C)(C_B)_2) + (4 \times C_B-(H)_3(C)) + (1 \times C_B-(C_d)(C_B)_2) + (1 \times SO_2-(C_d)(C_B)_3) + (1 \times C_d-(H)(C)) + (1 \times C_d-(H)_3(C)(C_d)) + (1 \times C_d-(H)_3(C)(C)(C_d)) + (1 \times C_d-(H)_3(C)(C)(C_d)) + (1 \times C_d-($	C_d -(H)(SO ₂))+	(1×C-((1×C _B -	$-(SO_2)(C_B)_2$	$\times C_B - (C)(C_B)_2$	(C_B) + $(1 \times$	C_d - $(H)(SO_2)) +$
Literature - Calculated = Residual	Reference		Literatu	re – Calculated	= Residual	Reference
0		Can about				
Gas phase $\Delta_t H^\circ = -229.80 -214.69 -15.11$	69MAC/MCN	Gas phase $\Delta_t H^\circ =$	- 60.00	-61.52	1.52	69MAC/MCN
	nv ·					
$\begin{aligned} &\textbf{1-Methyl-4-(2-methyl-2-propenylsulfonyl)benzene} \\ &(1 \times C - (H)_3(C)) + (1 \times C_B - (C)(C_B)_2) + (4 \times C_B - (H)_3(C)) + (1 \times C_B - (C)(C_B)_2) + (1 \times C_B - (C)(C_B)) + (1 \times C_$		(1×С-((1×С _в -	$-(C)(C_B)_2)+$	sulfone $0 \times C_{B}$ — $(H)(C_{B})_{2}$ $(1 \times SO_{2}$ — $(C_{d})(C_{B})$ $(1 \times C_{B}$ — $(C_{d})(C_{B})$	(C_B) + $(1 \times C_C)$	
Literature – Calculated = Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = -241.50 -238.29 -3.21$	69MAC/MCN	Gas phase $\Delta_t H^\circ =$	- 69.60	-66.37	-3.23	69MAC/MCN
Diphenyl sulfone $(10\times C_B-(H)(C_B)_2)+(2\times C_B-(SO_2)(C_B)_2)+(1\times S_B-(SO_2)(C_B)_2)+(1\times S$	$C_{12}H_{10}O_{2}S$ GO_{2} – $(C_{B})_{2})$	Diphenyl (+ (2×C _B -(SO ₂)	$(C_B)_2) + (2 \times$	C ₁₂ H ₁₀ O ₄ S ₂ SO ₂ -(SO ₂)(C _B))
Literature – Calculated = Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = -118.70 - 118.70$ 0.00	70COX/PIL	Gas phase $\Delta_t H^\circ =$	-481.30	-481.30	0.00	64МАС/ОНА
Solid phase $\Delta_t H^{\circ} = -225.00 -225.00 0.00$	61MAC/OHA2	Solid phas $\Delta_t H^\circ =$	e - 643.10	-643.10	0.00	64MAC/OHA
trans-Phenyl β -styryl sulfone $ (10 \times C_B - (H)(C_B)_2) + (1 \times C_B - (SO_2)(C_B)_2) + (1 \times C_d - (H)(C_B)) + (1 \times C_B - (H)(C_B)) + (1$						
Literature – Calculated = Residual	Reference					
Gas phase $\Delta_t H^{\circ} = -35.00 - 33.94 - 1.06$	69MAC/MCN					
Dibenzyl sulfone $ (10 \times C_B - (H)(C_B)_2) + (2 \times C_B - (C)(C_B)_2) + $	$C_{14}H_{14}O_2S$ $(H)_2(C_B)(SO_2)) +$ Reference					
Gas phase $\Delta_t H^{\circ} = -157.10 -162.80$ 5.70	61MAC/OHA					

TABLE 47. Sulfites (5)

TABLE 48. Sulfates (4)

Dimethyl sulfite $(2 \times C-(H)_3(C))+(2 \times O-(C)(SO))+(1 \times SO-(O)_2)$	C ₂ H ₆ O ₃ S	Dimethyl so (2×C-(I		× O-(C)(SO ₂))+(1×SO ₂ -(0	C₂H₄O₄S O)2)
Literature – Calculated = Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = -483.40 -482.72 -0.68$	69MAC/STE	Gas phase $\Delta_t H^\circ =$	- 687.00	-684.62	-2.38	69MAC/STE
Ethyl methyl sulfite $(2 \times C - (H)_3(C)) + (2 \times O - (C)(SO)) + (1 \times SO - (O)_2) (1 \times C - (H)_2(O)(C))$	C ₃ H ₈ O ₃ S +	Diethyl suli (2×C-(I (1×SO ₂ -	$H_{3}(C) + (2$	× C-(H)2(O)((C))+(2× O- ((C ₄ H ₁₀ O ₄ S C)(SO ₂)) +
Literature – Calculated = Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = -524.00 -515.62 -8.38$	69MAC/STE	Gas phase $\Delta_t H^\circ =$	-756.30	-750.42	-5.88	69MAC/STE
Diethyl sulfite $(2 \times C - (H)_3(C)) + (2 \times C - (H)_2(O)(C)) + (2 \times O - (C)(C)(C)) + (2 \times O - (C)(C)(C)) + (2 \times O - (C)(C)(C)(C)) + (2 \times O - (C)(C)(C)(C)(C) + (2 \times O - (C)(C)(C)(C)) + (2 \times O - (C)(C)(C)(C)(C)(C) + (2 \times O - (C)(C)(C)(C)(C)(C)(C)(C) + (2 \times O - (C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)($		1.	H) ₃ (C)) + (2 C)(SO ₂)) + (× C-(H) ₂ (C) ₂) 1 × SO ₂ -(O) ₂)	, , , , , , , , ,	. , , ,,
Literature - Calculated = Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = -552.20 -548.52 -3.68$	69MAC/STE	Gas phase $\Delta_t H^\circ =$	- 792.00	- 791.68	-0.32	69MAC/STE
Dipropyl sulfite $(2 \times C - (H)_2(C)) + (2 \times C - (H)_2(C)) + (2 \times C - (H)_2(C)) + (2 \times C - (H)_2(C))$ $(2 \times O - (C)(SO)) + (1 \times SO - (O)_2)$	C ₆ H ₁₄ O ₃ S)(C)) +		I) ₅ (C))+(4	× C-(H) ₂ (C) ₂) 1 × SO ₂ -(O) ₂)	+ (2×C-(H)₂(C ₈ H ₁₈ O ₄ S (O)(C)) +
Literature - Calculated = Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = -588.30 -589.78$ 1.48	69MAC/STE	Gas phase $\Delta_t H^\circ =$	- 828.90	- 832.94	4.04	69MAC/STE
Dibutyl sulfite $(2 \times C-(H)_3(C)) + (4 \times C-(H)_2(C)_2) + (2 \times C-(H)_2(O)_2) + (2 \times O-(C)(SO)) + (1 \times SO-(O)_2)$	C ₈ H ₁₈ O ₃ S)(C))+					
Literature - Calculated = Residual	Reference					

TABLE 49. Cyclic CHS (13)

TABLE 49. Cyclic CHS (13) - Continued

82.22 53.68 55.27 51.60	82.22 53.68 255.27 -49.41 96.95 -39.11 51.60 × C-(H) ₂ (C)(S) rsc), σ = 2 - Calculated = 61.00 69.33 285.22 -155.77 107.44 -43.34	0.00 0.00 0.00 0.00	S2GUT/SCO2 69STU/WES 69STU/WES 69STU/WES C3H6S C)2) + Reference 53SCO/FIN 69STU/WES 69STU/WES		140.16 207.82 140.16 207.82 140.16 207.82 140.16 207.82 140.16 140.1	-73.10 140.16 207.82 -369.48 37.06 -14.95 2×C-(H) ₂ (C)(See rsc), σ = 1 re - Calculated = -63.26 108.20 323.26 -390.35 53.12 -21.43	0.00 0.00 0.00	S4HUB/KAT 52HUB/FIN 52HUB/FIN 52HUB/FIN C ₅ H ₁₀ C) ₂) + Reference 54MCC/FIN 69STU/WES 69STU/WES
53.68 55.27 51.60 61.00 69.33	53.68 255.27 - 49.41 96.95 - 39.11 51.60 × C-(H) ₂ (C)(S) rsc), σ = 2 2 - Calculated = 61.00 69.33 285.22 - 155.77 107.44	0.00 0.00 0.00 0.00 = Residual	69STU/WES 69STU/WES 69STU/WES 63SUN C ₃ H ₆ S C) ₂) + Reference 53SCO/FIN 69STU/WES	$\Delta_f H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_f S^\circ =$ $\Delta_f G^\circ =$ $\ln K_f =$ Thiacycloh $(3 \times C - (1 \times This))$ Gas phase $\Delta_f H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_f S^\circ \Delta_f G^\circ =$ $\ln K_f =$	-73.10 140.16 207.82 mexane H) ₂ (C) ₂) + (2 acyclohexane Literatur -63.26 108.20 323.26	140.16 207.82 - 369.48 37.06 - 14.95 $2 \times C - (H)_2(C)(S$ ersc), $\sigma = 1$ re - Calculated = -63.26 108.20 323.26 - 390.35 53.12	0.00 0.00 0.00 0.00 = Residual	52HUB/FIN 52HUB/FIN C ₅ H ₁₀ C) ₂) + Reference 54MCC/FIN 69STU/WES
53.68 55.27 51.60 61.00 69.33	53.68 255.27 - 49.41 96.95 - 39.11 51.60 × C-(H) ₂ (C)(S) rsc), σ = 2 2 - Calculated = 61.00 69.33 285.22 - 155.77 107.44	0.00 0.00 0.00 0.00 = Residual	69STU/WES 69STU/WES 69STU/WES 63SUN C ₃ H ₆ S C) ₂) + Reference 53SCO/FIN 69STU/WES	$C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = \frac{1}{3}$ Thiacycloh (3 × C-((1 × This section of the context of th	140.16 207.82 nexane H) ₂ (C) ₂) + (2 acyclohexane Literatur -63.26 108.20 323.26	140.16 207.82 - 369.48 37.06 - 14.95 $2 \times C - (H)_2(C)(S$ ersc), $\sigma = 1$ re - Calculated = -63.26 108.20 323.26 - 390.35 53.12	0.00 0.00 0.00 0.00 = Residual	52HUB/FIN 52HUB/FIN C ₅ H ₁₀ C) ₂) + Reference 54MCC/FIN 69STU/WES
51.60 51.60 C() ₂) + (2 obutane Literature 61.00 69.33	255.27 -49.41 96.95 -39.11 51.60 \times C-(H) ₂ (C)(S) rsc), σ = 2 σ - Calculated = 61.00 69.33 285.22 -155.77 107.44	0.00 0.00 0.00 = Residual	69STU/WES 63SUN C ₃ H ₆ S C) ₂) + Reference 53SCO/FIN 69STU/WES	$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f = \frac{1}{3 \times C - (1 \times This)}$ Gas phase $\Delta_f H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_f G^{\circ} = \ln K_f = \frac{1}{3 \times C}$	207.82 nexane H) ₂ (C) ₂) + (2 acyclohexane Literatur -63.26 108.20 323.26	207.82 -369.48 37.06 -14.95 $2 \times C - (H)_2(C)(S$ e rsc), $\sigma = 1$ re - Calculated = -63.26 108.20 323.26 -390.35 53.12	0.00 (1) + (1 × S-(C) = Residual 0.00 0.00	C₅H₁₀ C)₂) + Reference 54MCC/FIN 69STU/WES
51.60 C()2) + (2) obutane Literature 61.00 69.33	-49.41 96.95 -39.11 51.60 \times C-(H) ₂ (C)(S) σ = 2 σ - Calculated = 61.00 69.33 285.22 -155.77 107.44	0.00)) + (1 × S-(C = Residual 0.00 0.00	63SUN C ₃ H ₆ S C) ₂) + Reference 53SCO/FIN 69STU/WES	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f = \frac{1}{3 \times C - (1 \times This}$ Gas phase $\Delta_f H^\circ = C_\rho^\circ = S^\circ = \Delta_f S^\circ - \Delta_f G^\circ = \ln K_f = \frac{1}{3 \times C}$	H) ₂ (C) ₂) + (2 acyclohexane Literatur - 63.26 108.20 323.26	-369.48 37.06 -14.95 $2 \times C - (H)_2(C)(S)$ $e rsc), \sigma = 1$ $re - Calculated = $ -63.26 108.20 323.26 -390.35 53.12	0.00 0.00	C ₅ H ₁₆ C) ₂) + Reference 54MCC/FIN 69STU/WES
c) + (2 c) + (2 c) cobutance Literature 61.00 69.33	96.95 - 39.11 51.60 × C-(H) ₂ (C)(S rsc), σ = 2 a - Calculated = 61.00 69.33 285.22 - 155.77 107.44	0.00 0.00	C ₃ H ₆ S C) ₂) + Reference 53SCO/FIN 69STU/WES	$\Delta_f G^\circ = \ln K_f = \frac{1}{100}$ Thiacycloh (3×C-(1×Thiacycloh) (1×Thiacycloh) (3×C-(1×Thiacycloh) (1×Thiacycloh) (3×C-(1×Thiacycloh) (1×Thiacycloh) (3×C-(1×Thiacycloh) (1×Thiacycloh) (3×C-(1×Thiacycloh) (3×C-(1×Thiacycloh) (1×Thiacycloh) (3×C-(1×Thiacycloh) (1×Thiacycloh) (3×C-(1×Thiacycloh) (1×Thiacycloh) (3×C-(1×Thiacycloh) (1×Thiacycloh) (3×C-(1×Thiacycloh) (1×Thiacycloh) (3×C-(1×Thiacycloh) (1×Thiacycloh) (3×C-(1×Thiacycloh) (3×C-(1×Thiacycloh) (1×Thiacycloh) (3×C-(1×Thiacycloh) (1×Thiacycloh) (3×C-(1×Thiacycloh) (1×Thiacycloh) (3×C-(1×Thiacycloh) (3×C-(1×	H) ₂ (C) ₂) + (2 acyclohexane Literatur -63.26 108.20 323.26	37.06 -14.95 $2 \times C - (H)_2(C)(S)$ $e r sc)$, $\sigma = 1$ re - Calculated = -63.26 108.20 323.26 -390.35 53.12	= Residual 0.00 0.00	Reference 54MCC/FIN 69STU/WES
c) + (2 c) + (2 c) cobutance Literature 61.00 69.33	-39.11 51.60 $\times C-(H)_2(C)(S)$ $rsc), \sigma = 2$ $- Calculated =$ 61.00 69.33 285.22 -155.77 107.44	0.00 0.00	C ₃ H ₆ S C) ₂) + Reference 53SCO/FIN 69STU/WES	In $K_f =$ Thiacycloh $(3 \times C - (1 \times This))$ Gas phase $\Delta_f H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_f S^\circ \Delta_f G^\circ =$ $\ln K_f =$	H) ₂ (C) ₂) + (2 acyclohexane Literatur -63.26 108.20 323.26	-14.95 $2 \times C - (H)_2(C)(S)$ $e rsc), \sigma = 1$ re - Calculated = -63.26 108.20 323.26 -390.35 53.12	= Residual 0.00 0.00	Reference 54MCC/FIN 69STU/WES
c) + (2 c) + (2 c) cobutance Literature 61.00 69.33	51.60 × C-(H) ₂ (C)(S) rsc), σ = 2 - Calculated = 61.00 69.33 285.22 - 155.77 107.44	0.00 0.00	C ₃ H ₆ S C) ₂) + Reference 53SCO/FIN 69STU/WES	Thiacycloh $(3 \times C - (1 \times This))$ Gas phase $\Delta_f H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} - \Delta_f G^{\circ} = InK_f = InK_f$	H) ₂ (C) ₂) + (2 acyclohexane Literatur -63.26 108.20 323.26	$2 \times \text{C-(H)}_2(\text{C})(\text{S} = \text{rsc}), \sigma = 1$ re – Calculated = -63.26 108.20 323.26 -390.35 53.12	= Residual 0.00 0.00	Reference 54MCC/FIN 69STU/WES
c) + (2 c) + (2 c) cobutance Literature 61.00 69.33	\times C-(H) ₂ (C)(S) rsc), $\sigma = 2$ \times - Calculated = 61.00 69.33 285.22 -155.77 107.44	0.00 0.00	C ₃ H ₆ S C) ₂) + Reference 53SCO/FIN 69STU/WES	$(3 \times C - (1 \times This))$ Gas phase $\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} - \Delta_{f}G^{\circ} = InK_{f} = 0$	H) ₂ (C) ₂) + (2 acyclohexane Literatur -63.26 108.20 323.26	-63.26 108.20 323.26 -390.35 53.12	= Residual 0.00 0.00	Reference 54MCC/FIN 69STU/WES
c) + (2 c) + (2 c) cobutance Literature 61.00 69.33	\times C-(H) ₂ (C)(S) rsc), $\sigma = 2$ \times - Calculated = 61.00 69.33 285.22 -155.77 107.44	0.00 0.00	C ₃ H ₆ S C) ₂) + Reference 53SCO/FIN 69STU/WES	$(3 \times C - (1 \times This))$ Gas phase $\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} - \Delta_{f}G^{\circ} = InK_{f} = 0$	H) ₂ (C) ₂) + (2 acyclohexane Literatur -63.26 108.20 323.26	-63.26 108.20 323.26 -390.35 53.12	= Residual 0.00 0.00	Reference 54MCC/FIN 69STU/WES
C) ₂) + (2 lobutane Literature 61.00 69.33	61.00 69.33 285.22 -155.77 107.44	= Residual 0.00 0.00	Reference 53SCO/FIN 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} - \Delta_{t}G^{\circ} = InK_{t} =$	-63.26 108.20 323.26	-63.26 108.20 323.26 -390.35 53.12	0.00	54MCC/FIN 69STU/WES
61.00 69.33	61.00 69.33 285.22 155.77 107.44	0.00	53SCO/FIN 69STU/WES	$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} - \Delta_{t}G^{\circ} = InK_{t} =$	- 63.26 108.20 323.26	108.20 323.26 -390.35 53.12	0.00	69STU/WES
61.00 69.33	61.00 69.33 285.22 155.77 107.44	0.00	53SCO/FIN 69STU/WES	$C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} - \Delta_{f}G^{\circ} = \ln K_{f} =$	108.20 323.26	108.20 323.26 -390.35 53.12	0.00	69STU/WES
69.33	69.33 285.22 155.77 107.44	0.00	69STU/WES	$S^{\circ} = \Delta_{f}S^{\circ} - \Delta_{f}G^{\circ} = \ln K_{f} =$	323.26	323.26 - 390.35 53.12		
69.33	69.33 285.22 155.77 107.44	0.00	69STU/WES	$\Delta_f S^\circ - \Delta_f G^\circ = \ln K_f =$		-390.35 53.12	0.00	69STU/WE
69.33	69.33 285.22 155.77 107.44	0.00	69STU/WES	$\Delta_f G^\circ = In K_f =$		53.12		
69.33	69.33 285.22 155.77 107.44	0.00	69STU/WES	$lnK_f =$				
	285.22 155.77 107.44					-21.43		· · · · · · · · · · · · · · · · · · ·
85.22	155.77 107.44	0.00	69STU/WES	Liquid pha				<u> </u>
	107.44			Liquid pha				
				Liquid pha				
	-43.34				ise			
				$\Delta_{\rm f}H^{\circ} =$	-106.00	- 106.00	0.00	54MCC/FIN
				$C_p^{\circ} =$	163.30	163.30	0.00	54MCC/FIN
				S° =	218.24	218.24	0.00	54MCC/FIN
				$\Delta_{f}S^{\circ} =$		- 495.37		
25.10	25.10	0.00	54HUB/KAT	$\Delta_t G^\circ =$		41.69		
13.39	113.39	0.00	53SCO/FIN	$lnK_f =$		-16.82		
84.93	184.93	0.00	53SCO/FIN					
	- 256.06							
	101.44							
	- 40.92			Thiacycloh	•			C6H12S
						$2 \times C - (H)_2(C)(S)$ ne rsc), $\sigma = 1$))+(1× 5- (C	·)2)+
		S))+(1×S-(C	C ₄ H ₈ S		Literatur	re – Calculated =	Residual	Reference
lopentan	e rsc), $\sigma = 2$			Gas phase				
Literatur	e – Calculated =	= Residual	Reference	$\Delta_{\rm f}H^{\circ} =$	-61.34	-61.34	0.00	69STU/WES
				$C_p^{\circ} =$	124.60	124.60	0.00	69STU/WES
				S° =	361.92	361.92	0.00	69STU/WES
				$\Delta_f S^\circ =$		- 488.00		
34.20	-34.20	0.00	52HUB/FIN	$\Delta_t G^\circ =$		84.16		
90.88	90.88	0.00	69STU/WES	$\ln K_{\rm f} =$		-33.95		
309.36	309.36	0.00	69STU/WES	-				
	-267.94							
	45.69			T 1 . 1 4 . 1 . 1				
				Liquid bha	ise			69STU/WES
Clo Li -3 9	(1) ₂) + (2 pentand terature 4.20 0.88	(2) ₂) + (2 × C-(H) ₂ (C)(S) pentane rsc), σ = 2 terature – Calculated = 4.20 – 34.20 0.88 90.88 9.36 309.36 – 267.94	$(2)_2 + (2 \times C - (H)_2(C)(S)) + (1 \times S - (G)_2(C)(S)) + (1 \times G)_2(C)(S) + (1 \times G)_2(C)(C)(S) + (1 \times G)_2(C)(C)(S) + (1 \times G)_2(C)(C)(S) + (1 \times G)_2(C)(C)(C)(S) + (1 \times G)_2(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)($	$(2)_2 + (2 \times C - (H)_2(C)(S)) + (1 \times S - (C)_2) + (1 \times S - (C)_2$	$C(x) + (2 \times C - (H)_2(C)(S)) + (1 \times S - (C)_2) + C(x)_2 + C(x)_3 + C(x)_4 + C(x)_5 + C(x)_$	$\begin{array}{c} (C_{1})_{2} + (2 \times C - (H)_{2}(C)(S)) + (1 \times S - (C)_{2}) + \\ (C_{1})_{2} + (2 \times C - (H)_{2}(C)(S)) + (1 \times S - (C)_{2}) + \\ (C_{2})_{3} + (2 \times C - (H)_{2}(C)(S)) + (1 \times S - (C)_{2}) + \\ (C_{2})_{4} + (2 \times C - (H)_{2}(C)(S)) + (1 \times S - (C)_{2}) + \\ (C_{2})_{5} + (2 \times C - (H)_{2}(C)(S)) + (1 \times S - (C)_{2}) + \\ (C_{2})_{5} + (2 \times C - (H)_{2}(C)(S)) + (1 \times S - (C)_{2}) + \\ (C_{2})_{5} + (2 \times C - (H)_{2}(C)(S)) + (1 \times S - (C)_{2}) + \\ (C_{2})_{5} + (2 \times C - (H)_{2}(C)(S)) + (1 \times S - (C)_{2}) + \\ (C_{2})_{5} + (2 \times C - (H)_{2}(C)(S)) + (1 \times S - (C)_{2}) + \\ (C_{2})_{5} + (2 \times C - (H)_{2}(C)(S)) + (1 \times S - (C)_{2}) + \\ (C_{2})_{5} + (2 \times C - (H)_{2}(C)(S)) + (1 \times S - (C)_{2}) + \\ (C_{2})_{5} + (2 \times C - (H)_{2}(C)(S)) + (1 \times S - (C)_{2}) + \\ (C_{2})_{5} + (2 \times C - (H)_{2}(C)(S)) + (1 \times S - (C)_{2}) + \\ (C_{2})_{5} + (2 \times C - (H)_{2}(C)(S)) + (2 \times C - (H)_{2}(C)(S) + (2 \times C - (H)_{2}(C)(S)) + \\ (C_{2})_{5} + (2 \times C - (H)_{2}(C)(S)) + (2 \times C - (H)_{2}(C)(S) + (2 \times C - (H)_{2}(C)(S)) + \\ (C_{2})_{5} + (2 \times C - (H)_{2}(C)(S)) + (2 \times C - (H)_{2}(C)(S) + (2 \times (H)_{2}(C)(S)) + \\ (C_{2})_{5} + (2 \times (H)_{2}(C)(S)) + (2 \times (H)_{2}(C)(S) + (2 \times (H)_{2}(C)(S)) + (2 \times (H)_{2}(C)(S) + (2 \times (H)_{2}(C)(S)) + \\ (C_{2})_{5} + (2 \times (H)_{2}(C)(S)) + (2 \times (H)_{2}(C)(S) + (2 \times (H)_{2}(C)(S)) + (2 \times (H$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

TABLE 49. Cyclic CHS (13) - Continued

TABLE 49. Cyclic CHS (13) - Continued

Thiophene	C ₄ H ₄ S
$(4 \times C_B - (H)(C_B)_2) + (1 \times S - (C_B)_2) + (1 \times Thiophene rsc), \sigma =$	2

	Literatur	Reference						
Gas phase								
$\Delta_f H^\circ =$	114.30	114.30	0.00	49WAD/KNO				
Cp -	72.89	72.89	0.00	69STU/WES				
S°=	278.86	278.86	0.00	69STU/WES				
Δ ₆ S° =		-37.30						
$\Delta_r G^\circ =$		125.42						
lnK_f -		- 50.59						

2-Methylthiophene $C_sH_6S \\ (3\times C_B-(H)(C_B)_2)+(1\times C_B-(C)(C_B)_2)+(1\times C-(H)_3(C))+\\ (1\times S-(C_B)_2)+(1\times Thiophene \ rsc), \ \sigma=3$

	Literatur	Reference		
Gas phase				
Δ _r H° ~	83.68	81.87	1.81	69STU/WES
$C_{\rho}^{\circ} =$	95.40	94.76	0.64	69STU/WES
s° =	320.58	318.89	1.69	69STU/WES
$\Delta_t S^\circ =$		- 133.58		
$\Delta_{c}G^{\circ} =$		121.70		
$lnK_f =$		- 49.09		

	Literatur	Reference		
Gas phase				
$\Delta_f H^\circ =$	82.80	81.87	0.93	69STU/WES
$C_p^{\circ} =$	94.85	94.76	0.09	69STU/WES
S° =	321.29	318.89	2.40	69STU/WES
$\Delta_t S^\circ =$		- 133.58		
$\Delta_t G^\circ =$		121.70		
$lnK_f =$		-49.09		

2-Methyl thiolane $\begin{array}{c} C_5H_{10}S \\ (2\times C-(H)_2(C)_2) + (1\times C-(H)_2(C)(S)) + (1\times C-(H)(C)_2(S)) + \\ (1\times C-(H)_3(C)) + (1\times S-(C)_2) + (1\times Thiacyclopentane\ rsc) \end{array}$

	Literatur	Reference		
Gas phase $\Delta_t H^\circ = C_\rho^\circ =$	- 64.20	- 59.17 116.00	-5.03	72GOO2

2-Methyl thiolane (Continued)	C5H10S
$(2 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)(S)) + (1 \times C - (H)(C)_2(S)) - (1 \times C - (H)_2(C)_2(S)) + (1 \times C - (H)_2(C)_2(S)_2(S)) + (1 \times C - (H)_2(C)_2(S)_2(S)_2(S)_2(S)_2(S)_2(S)_2(S)_2(S$	+
$(1 \times C - (H)_3(C)) + (1 \times S - (C)_2) + (1 \times Thiacyclopentane rsc)$	

	Literatu	Reference		
Liquid ph				
$\Delta_r H^o -$	-105.40	-100.01	- 5.39	72GOO2
$C_p^{\circ} =$	171.80	170.24	1.56	74MES/FIN
S° =	245.31	233.42	11.89	74MES/FIN
$\Delta_f S^\circ =$		- 480.19		
$\Delta_t G^\circ$ –		43.16		
$lnK_{f} =$		- 17.41		

3-Methyl thiolane $\begin{array}{c} C_5H_{10}S \\ (1\times C-(H)_2(C)_2) + (1\times C-(H)_3(C)) + (1\times C-(H)(C)_3) + \\ (2\times C-(H)_2(C)(S)) + (1\times S-(C)_2) + (1\times Thiacyclopentane\ rsc) \end{array}$

	Literature – Calculated = Residual						
Gas phase	1						
$\Delta_f H^\circ =$	-60.50	-57.00	-3.50	72GOO2			
$C_p^{\circ} =$		113.80					
Liquid pha	ase	· · · · · · · · · · · · · · · · · · ·					
Liquid pha Δ _t H° =	ase - 102.70	-99.75	- 2.95	72GOO2			
		- 99.75 167.60	- 2.95 4.20	72GOO2 74MES/FIN			
$\Delta_f H^\circ =$	-102.70						
$\Delta_f H^\circ = C_p^\circ =$	- 102.70 171.80	167.60	4.20	74MES/FIN			
$\Delta_{\rm f} H^{\circ} = C_{\rm p}^{\circ} = S^{\circ} =$	- 102.70 171.80	167.60 234.85	4.20	74MES/FIN			

Cyclopentyl methyl sulfide	C ₆ H ₁₂ S
$(1 \times C - (H)_3(S)) + (1 \times S - (C)_2) + (4 \times C - (H)_2(C)_2) +$	
$(1 \times C - (H)(C)_2(S)) + (1 \times Cyclopentane (sub) rsc)$	

	Literatu	Reference		
Gas phase Δ _f H° =	e -64.70	-64.12	-0.58	72GOO2
$C_p^a =$		132.35		
Liquid ph $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	109.80 192.92 285.47	- 103.19 197.77 282.66 - 567.26	-6.61 -4.85 2.81	72GOO2 74MES/TOD 74MES/TOD
$\Delta_i G^{\circ} \sim$		65.94		

TABLE 49. Cyclic CHS (13) - Continued

TABLE 50. Fluorides (46)

(1×C-(H)	C_d) + (1 × $_2$ (C)(C_d)) +	C_{d} -(H)(S)) + ((1 × C-(H) ₂ (C		C ₄ H ₆ S	Fluoromethane; Methyl fluoride $(1 \times C - (H)_3(F), \text{ methyl fluoride}), \sigma = 3$ Literature – Calculated = Residual			CH ₃ I Reference	
(1×2,3-Dil	•	hene rsc) : Calculated=	: Recidual	Reference	Literatui	re – Calculated :	= Kesidual	Reference	
Gas phase $\Delta_f H^\circ =$	90.70	90.70	0.00	62DAV/SUN	Gas phase $\Delta_t H^\circ = -247.00$ $C_\rho^\circ = 37.49$ $S^\circ = 222.80$ $\Delta_t S^\circ = \Delta_t G^\circ =$	-247.00 37.49 222.80 -80.14	0.00 0.00 0.00	85LIA/KAR 69STU/WES 69STU/WES	
2,5-Dihydroth (1×S-(C) ₂ (1×2,5-Dil)+(2×C-	(H) ₂ (C _d)(S)) +	(2×C _d -(H)(C₄H ₆ S	$\ln K_{\rm f} =$	-223.11 90.00			
(17,2,5,2,2)	•	- Calculated =	= Residual	Reference	Fluoroethane $(1 \times C - (H)_3(C)) + (1$	× C-(H) ₂ (C)(F))), σ = 3	C ₂ H ₅ I	
Gas phase			*****		Literatur	e – Calculated =	- Residual	Reference	
$\Delta_t H^\circ =$ Liquid phase $\Delta_t H^\circ =$	86.90 47.00	47.00	0.00	62DAV/SUN 62DAV/SUN	Gas phase $\Delta_t H^\circ = -261.50$ $C_p^\circ = 59.04$ $S^\circ = 264.93$ $\Delta_t S^\circ = \Delta_t G^\circ = 10K_f = 100$	- 263.38 59.39 264.99 - 174.26 - 211.42 85.29	1.88 -0.35 -0.06	69STU/WES 69STU/WES 69STU/WES	
				3	1-Fluoropropane (1×C-(H) ₃ (C))+(1 Literatur	× C-(H) ₂ (C) ₂) + re – Calculated =		$C_3H_{7}I$ (C)(F)), $\sigma = 3$ Reference	
					Gas phase $\Delta_t H^{\circ} = -285.90$ $C_p^{\circ} = 82.63$ $S^{\circ} = 304.22$ $\Delta_t S^{\circ} = \Delta_t G^{\circ} = 10K_f = 100$	- 284.01 82.28 304.15 - 271.41 - 203.09 81.92	- 1.89 0.35 0.07	56LAC/KIA2 69STU/WES 69STU/WES	
					2-Fluoropropane (2×C-(H) ₃ (C))+(1 (2×-CH ₃ corr (terti	ary))		C ₃ H ₇ F	
					Gas phase $\Delta_t H^\circ = -293.50$ $C_p^\circ = 82.01$	- 293.50 82.01	0.00 0.00	S6LAC/KIA2 69STU/WES	

1,1-Diffuoroethane $(1 \times C - (H)_3(C)) + (1 \times C - (H)(C)(F)_2), \sigma = 3$		$C_2H_4F_2$	Hexadecaflu (2×C-(C		e × C-(C) ₂ (F) ₂)		C7F16		
	Literature	e – Calculated	= Residual	Reference		Literatui	e – Calculated	l = Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	- 497.00 67.95 282.51	497.00 67.95 282.51	0.00 0.00 0.00	68KOL/SHT 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ = -C_p^\circ =$	- 3383.60	- 3404.57 313.08	20.97	510LI/GRI
$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-192.80 -439.52 177.30			Liquid phas $\Delta_t H^{\circ} = -$		- 3419.99	- 0.01	59GOO/DOU
1,1,1-Trifluo (1 × C–(H		× C-(C)(F)3),	$\sigma = 9$	C ₂ H ₃ F ₃	Tetrafluoro	ethylene F) ₂), σ = 4			C₂F.
	Literatur	e – Calculated	= Residual	Reference		Literatui	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	744.60 78.45 287.27	-716.07 78.72 287.27 -224.09 -649.26 261.91	-28.53 -0.27 0.00	65KOL/MAR 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 659.80 80.50 299.95	- 659.80 78.86 299.73 - 117.11 - 624.88 252.07	0.00 1.64 0.22	56SCO/GOO 69STU/WES 69STU/WES
1,1,2-Trifluo (1 × C-(H	(C)(F) ₂)+	- (1 × C-(H) ₂ (C		C ₂ H ₃ F ₃	Fluoroethyle (1×C _d -(1	H)(F))+(1	× C _d -(H) ₂) e – Calculated	= Residual	C₂H₃F Reference
								- Nosiduii	
$C_{\rho}^{\circ} = S^{\circ} =$	– 730.70	-675.86 75.88 311.12	- 54.84	56LAC/KIA	Gas phase $\Delta_t H^\circ = C_t^\circ =$	- 138.80	- 138.80 49.83	0.00	70KOL/PAP
$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-200.24 -616.16 248.55			1,1-Difluoro (1×C _d -(1		C_d - $(F)_2$), $\sigma =$	2	C ₂ H ₂ F ₂
Hexafluoroe	thane ()(F) ₃), σ =	- 1 8		C ₂ F ₆	-	Literatur	e – Calculated	= Residual	Reference
	,,,,,	re – Calculated	= Residual	Reference	$C_p^{\circ} =$	-334.00 59.16	-303.58 60.81	-30.42 -1.65	56NEU/MAR 69STU/WES
Gas phase $\Delta_t H^\circ = -\frac{C_t^\circ - S^\circ}{S^\circ} = \frac{1}{2}$	-1343.10 106.40 322.08	-1347.62 105.98 332.41	4.52 0.42 -10.33	66SIN 69STU/WES 69STU/WES	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} -$	265.18	265.39 - 79.35 - 279.92 112.92	-0.21	69STU/WES
$\Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} -$		- 287.12 - 1262.02 509.09							

TABLE 50. Fluorides (46) - Continued

Frifluoroet (1×C _d -($\times C_{\mathfrak{a}}-(F)_2), \sigma =$	= 1	C ₂ HF ₃		$-(F)(C_B)_2)-$	$+(2\times C_B-(C_B)_3)$)+(8× <i>ortho</i> c	$C_{12}F_1$ orr- $(F)(F)$) +
	Literatur	e – Calculated	= Residual	Reference	(2×ortho	corr-(F)(l	('))		
				· · · · · · · · · · · · · · · · · · ·		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$	490.40 69.20 292.62	495.02 67.88 292.87 87.92 468.81	4.62 1.32 -0.25	62KOL/MAR 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 1263.20	- 1586.08 287.24	322.88	79PRI/SAP2
$\ln K_f =$		189.11			Liquid pha	se			
					$\Delta_{\mathbf{f}}H^{\circ} = C_{\mathbf{p}}^{\circ} =$		- 1661.58 405.04		
3.3.3-Triflu	oropropene			C ₃ H ₃ F ₃					
		C_{d} -(H)(C))+($1 \times C - (C)(F)_3$		Solid phase $\Delta_t H^\circ = -$		- 1685.94	337.84	79PRI/SAP2
	Literatu	re – Calculated	= Residual	Reference	$C_p^{\circ} = S^{\circ} =$	1540.10	317.06 385.90	337.04	/91 KI/3AI 2
					$\Delta_{\rm r} S^{\circ} =$		-696.39		
Gas phase $\Delta_i H^\circ = C_p^\circ =$	-614.20	-611.17 93.11	-3.03	67KOL/MAR	$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = $		- 1478.31 596.34		
******					Fluorobenz				C₄H₅I
Hexafluore		(6× <i>ortho</i> corr-	$(F)(F), \sigma = 1$	C ₆ F ₆	$(1 \times C_B - ($	$(F)(C_B)_2) +$	$(5 \times C_B - (H)(C_E)$	$(\alpha_1)_2$), $\sigma = 2$	
(re – Calculated		Reference		Literatu	re – Calculated	= Residual	Reference
		- Culturated			<u> </u>	,			
Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	- 955.60 156.61 383.21	- 962.16 156.60 384.46 - 258.03 - 885.23 357.10	6.56 0.01 -1.25	65COU/GRE 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = L_t G^\circ = L_t K_t = L_t K_t = L_t K_t K_t K_t K_t K_t K_t K_t K_t K_t K$	-116.00 94.43 302.63	-112.21 94.15 303.31 -158.90 -64.83 26.15	- 3.79 0.28 - 0.68	56SCO/MCC 69STU/WES 69STU/WES
Liquid pha	ase				Liquid pha Δ _t H° =	- 150.60	- 150.40	- 0.20	56SCO/GOO
$ \Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} - InK_{f} = S^{\circ} $	- 991.30 221.58 280.79	- 997.20 222.54 325.14 - 317.35 - 902.58 364.10	5.90 0.96 44.35	69COX/GUN 65COU/GRE 65COU/GRE	$C_p^o = S^o = S_t^o = \Delta_t G^o = InK_t = S_t^o = S_t^$	146.36 205.94	150.49 198.54 - 263.67 - 71.79 28.96	- 4.13 7.40	56SCO/MCC 56SCO/MCC
$(5 \times C_{B}$	(F)(C _B) ₂)+ o corr-(F)(C	nethyl)benzene $(1 \times C_B - (C)(C_B + (C_B + C_B)) + (4 \times orthogonal)$	o corr-(F)(F)		$(1 \times C_{B} - ($	$(F)(C_B)_2) + H_{3}(C), \sigma$	tene; p-Fluoroto $(4 \times C_B - (H)(C_B = 6)$ re - Calculated	$(1)_2$ + $(1 \times C_{B}$ - $($	C_7II_7F $C)(C_B)_2) +$ Reference
	Literatu	re – Calculated	= Kesidual	Reference	-				
Gas phase $\Delta_l H^\circ = C_p^\circ =$	- 1268.60	- 1268.85 192.55	0.25	73KRE/PRI	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	-147.50 116.15 339.53	- 144.64 116.02 337.57 - 260.95	-2.86 0.13 1.96	62SCO/MES 69STU/WES 69STU/WES
Liquid ph		4000 ===	0.50	#ATT	$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} = $		- 66.84 26.96		
$\Delta_t H^\circ =$	- 1310.20	- 1309.50	-0.70	73KRE/PRI	-•				

$(1 \times C_B - (1 \times C_B))$	methylbenze $F(C_B)_2 + (\sigma + \sigma)_3(C)$	ne; p -Fluoroto 4 × C _B -(H)(C _B)	oluene (Contii $(C_B - (1 \times C_B - (1 \times C_B)))$	aued) C_7H_7F $C)(C_B)_2) +$	1,4-Difluor ($4 \times C_{B}$ -		$(2 \times C_B - (F)(C_E)$	$(s)_2), \sigma = 2$	C ₆ H ₄ F ₂
(1×C-(n		e – Calculated :	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
					C 1				
Liquid phas	se.				Gas phase $\Delta_t H^\circ =$	- 306.70	-307.28	0.58	62GOO/LAC
	186.90	- 187.01	0.11	62GOO/LAC	$C_n^{\circ} =$	106.90	106.64	0.26	69STU/WES
$C_p^{\circ} =$		174.39			S° =	315.60	322.52	-6.92	69STU/WES
S° =		233.47			$\Delta_{\mathbf{f}}S^{\circ} =$		- 175.75		
$\Delta_{\rm f} S^{\circ} =$		-365.05			$\Delta_i G^{\circ} =$		-254.88		
$\Delta_t G^{\circ} =$		-78.17			$lnK_f =$		102.82		
$lnK_f =$		31.53							
					Liquid pha				
					$\Delta_i H^\circ =$	- 342.42	- 349.76	7.34	62GOO/LAC
1,2-Difluore				C ₆ H ₄ F ₂	$C_p^o =$	160.70	164.90	-4.20	50UEB/ORT
		$(2 \times C_B - (F)(C_B)$	1)2)+		S° =		223.86		
(1×ortho	corr-(F)(F)), $\sigma = 2$			$\Delta_{\mathbf{f}}S^{\circ} =$		-274.40		
					$\Delta_f G^\circ =$		- 267.95		
	Literatur	e – Calculated	= Residual	Reference	$lnK_f =$		108.09		
Gas phase									
$\Delta_f H^\circ =$	- 293.80	286.38	-7.42	63SCO/MES	2.2'-Diffue	orobiphenyl			$C_{12}H_8F_2$
$C_p^{\circ} =$	106.52	106.64	-0.12	69STU/WES			$(2 \times C_B - (F)(C_B)$	() ₂) + (2 × C ₂ −4	
S° =	320.03	322.52	-2.49	69STU/WES		io corr-(F)(I		(2) · (2 · · OB ·	(- B)3) .
$\Delta_e S^\circ =$	520.05	- 175.75	2	0,010,1120	(27.07	(1)(1	"		
$\Delta_f G^\circ =$		- 233.98				Literatu	re - Calculated	= Residual	Reference
$lnK_f =$		94.39							
					Gas phase	;			
Liquid pha	ise				$\Delta_{\rm f} H^{\circ} =$	-200.80	-200.72	-0.08	64SMI/GOR
$\Delta_{\rm f}H^{\circ} =$	-330.16	- 324.76	-5.40	62GOO/LAC	$C_p^{\circ} =$		187.32		
$C_p^{\circ} =$	159.03	164.90	-5.87	63SCO/MES					
S° =	222.59	223.86	-1.27	63SCO/MES					
$\Delta_t S^\circ =$		-274.40			Liquid pha	ase			
$\Delta_t G^\circ =$		-242.95			$\Delta_t H^\circ =$		~274.70		
$lnK_f =$		98.00			$C_p^{\circ} =$		289.76		
					Solid phas	20			
1,3-Diffuor	whenzene			C ₆ H ₄ F ₂	$\Delta_t H^\circ =$	- 295.80	-293.70	-2.10	64SMI/GOR
•		$(2 \times C_R - (F)(C_B)$	7-7-1	C61141 2	$C_p^{\circ} =$	275.00	221.70	2.10	045MI/OOK
	corr-(F)(F		3,72,7 .		S° =		249.58		
(,,, -			$\Delta_{\rm f} S^{\circ} =$		- 544.27		
	Literatu	re - Calculated	= Residual	Reference	$\Delta_t G^{\circ} =$		-131.43		
					$lnK_f =$		53.02		
Gas phase									
$\Delta_{\mathbf{f}}H^{\circ} =$	-309.20	-307.28	-1.92	62GOO/LAC					
$C_p^{\circ} =$	106.27	106.64	-0.37	69STU/WES		probiphenyl			$C_{12}H_8F_2$
S° =	320.37	322.52	-2.15	69STU/WES	$(8 \times C_B -$	$-(H)(C_B)_2) +$	$(2 \times C_B - (F)(C_B$	$(2) + (2 \times C_{B} - (2 \times C_{B}))$	
$\Delta_{\rm f} S^{\circ} =$		- 175.75					_		
$\Delta_t G^\circ =$		-254.88				Literatu	re – Calculated	= Residual	Reference
$\ln K_{\ell} =$		102.82							
Liquid pha					Gas phase		200 72	2.40	CARNATIONE
LAGUIGI DISA		242 76	0.27	GCOOT AC	$\Delta_{\rm f}H^{\circ} =$	-205.30	-208.72	3.42	64SMI/GOR
	-344.13 159.12	343.76 164.90	0.37 5.78	62GOO/LAC	$C_r^{\circ} =$		187.32		
$\Delta_t H^\circ =$	137.14	223.86	-5.78 -0.02	70MES/FIN					· · · · · · · · · · · · · · · · · · ·
$\Delta_t H^\circ = C_p^\circ =$	222 04	443.00	- 0.02	70MES/FIN					
$\Delta_t H^\circ = C_p^\circ = S^\circ =$	223.84				Liquid -L.	ana			
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	223.84	-274.40			Liquid pha	ase	202 70		
$\Delta_t H^\circ = C_p^\circ = S^\circ =$	223.84				Liquid phate $\Delta_t H^\circ = C_p^\circ =$	ase	-282.70 289.76		

TABLE	50.	Fluorides	(46) -	Continued

(8×C _B −(H)(C _B) ₂)+($2 \times C_B - (F)(C_B)$) ₂) + (2 × C _B -(C _B) ₃)	(8×C _B (H)(C _B) ₂)+	$(2 \times C_B - (F)(C_1)$	$_{3})_{2}) + (2 \times C_{B} - ($	(C _B) ₃)
	Literature	e – Calculated =	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Solid phase	206 50	_ 301 70	5.20	64SML/GOD	Liquid phas $\Delta_t H^\circ =$	se	_ 673 48		
$\Delta_i H^\circ = -C_p^\circ =$. 290.30	-301.70 221.70	3.20	64SMI/GOR	$C_p^{\circ} =$	189.91	- 673.48 193.72	-3.81	73AND/MAR
$S^{\circ} =$		249.58			S° =	256.10	274.50	- 18.40	73AND/MAR
$\Delta_f S^\circ =$		-544.27			$\Delta_{f}S^{\circ} =$		-295.88	100	/U. I. \D/\\II \I
$\Delta_{\rm f}G^{\circ} =$		-139.43			$\Delta_{\mathfrak{l}}G^{\circ} =$		-585.26		
lnK _f =		56.24		n#+	$lnK_f =$		236.09		
· •									
(Trifluorome ($5 \times C_B$ –(H	•	ne $(1 \times C_B - (C)(C_B)$) ₂) + (1 × C-(0	$C_7H_5F_3$ $C_B)(F)_3)$			$(4 \times C_B - (F)(C_F)$	3)2)+(2×ortho	C_6H_2F corr-(F)(F)) +
	Literatur	e – Calculated =	= Residual	Reference	.`		e – Calculated	= Residual	Reference
Gas phase	500 TA	50W 10	0.00	509C (A/D/A) I	Constant				
$\Delta_{\mathbf{f}}H^{\circ} = -$ $C_{p}^{\circ} =$	- 599.10	599.10 130.10	0.00	59SCO/DOU	Gas phase $\Delta_t H^\circ =$		-655.62		
C _p =		130.10			$C_p^{\circ} =$		131.62		
Liquid phase $\Delta_t H^\circ = -$: - 636.70	-636.70	0.00	64GOO/LAC	Liquid phas $\Delta_t H^\circ =$	se	696.49		
					$\Delta \epsilon H^{-} =$		- 686.48		
					-	100.20	103 72	_ 3.43	73 A NID /M A D
					$C_p^{\circ} =$	190.29 257.32	193.72 274.50	- 3.43 - 17.18	73AND/MAR 73AND/MAR
1,2,4,5-Tetra	fluorobenz	ene		C ₆ H ₂ F ₄	$C_p^{\circ} = S^{\circ} =$	190.29 257.32	193.72 274.50 - 295.88	-3.43 -17.18	73AND/MAR 73AND/MAR
)2)+(2×ortho	$C_6H_2F_4$ $C_6F_7(F)$	$C_p^{\circ} =$		274.50		
$(2 \times C_{B}-(1$		$(4 \times C_B - (F)(C_B)$) ₂)+(2× <i>ortho</i>		$C_p^{\circ} = S^{\circ} = \Delta_f S^{\circ} =$		274.50 -295.88		•
	I)(C _B) ₂)+(corr-(F)(F)	$(4 \times C_B - (F)(C_B)$			$C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = 0$		274.50 - 295.88 - 598.26		•
(2×C _B -(F (2×meta	I)(C _B) ₂)+(corr-(F)(F)	$(4 \times C_B - (F)(C_B))$		corr-(F)(F))+	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = 1$ 1-Fluoro-3-(257.32	274.50 - 295.88 - 598.26 241.34	- 17.18	73AND/MAR C₁H₄F
(2×C _B -(F) (2×meta o	I)(C _B) ₂)+(corr-(F)(F)	(4×C _B -(F)(C _B))) e - Calculated =		corr-(F)(F))+	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = 1$ 1-Fluoro-3-($(4 \times C_B - (1 + C_b)^2)$	257.32 (trifluorome H)(C _B) ₂)+	274.50 - 295.88 - 598.26 241.34 	- 17.18	73AND/MAR C₁H₄F
(2×C _B -(F) (2×meta c	I)(C _B) ₂)+(corr-(F)(F)	$(4 \times C_B - (F)(C_B))$		corr-(F)(F))+	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = 1$ 1-Fluoro-3-($(4 \times C_B - (1 + C_b)^2)$	257.32 (trifluorome H)(C_B) ₂) + (1	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _B × meta corr-(F)	-17.18 -17.18 -17.18 -17.18 -17.18 -17.18	73AND/MAR $C_7H_4F_1$ $C)(C_B)_2) +$
$(2 \times C_B - (F_C)^2)$ $(2 \times meta)$ Gas phase $\Delta_t H^\circ =$	I)(C _B) ₂)+(corr-(F)(F)	(4×C _B -(F)(C _B)) e - Calculated = -655.62		corr-(F)(F))+	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1-\text{Fluoro-3-}(4 \times C_B - C_t)}{4 \times C_B - C_t}$	257.32 (trifluorome H)(C_B) ₂) + (1	274.50 - 295.88 - 598.26 241.34 	-17.18 -17.18 -17.18 -17.18 -17.18 -17.18	73AND/MAR C7H4F
$(2 \times C_B - (F + F))$ $(2 \times meta + G + F)$ $C_P = C_P = C_P$ Liquid phase	I)(C _B) ₂) + (corr-(F)(F) Literatur	(4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62	= Residual	Reference	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1-\text{Fluoro-3-}(4 \times C_B - C_t)}{4 \times C_B - C_t}$	257.32 (trifluorome H)(C_B) ₂) + (1	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _B × meta corr-(F)	-17.18 -17.18 -17.18 -17.18 -17.18 -17.18	73AND/MAR C ₇ H ₄ F C)(C _B) ₂) +
$(2 \times C_B - (H + (2 \times meta)))$ $Gas phase$ $\Delta_t H^\circ = C_p^\circ =$	H)(C _B) ₂) + (corr-(F)(F) Literatur	(4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48	= Residual	Reference 78HAR/HEA	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1-\text{Fluoro-3-}(4 \times C_B - C)}{(1 \times C - C)}$	257.32 (trifluorome H)(C_B) ₂) + (1 C_B) ₃) + (1	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _E × meta corr-(F)	-17.18 $(a)_{2} + (1 \times C_{B} - (CF3))$ = Residual	73AND/MAR C_7H_4F $C)(C_B)_2) +$ Reference
Gas phase $C_{p}^{\mu} = C_{p}^{\mu} = C_{p}^{\mu}$ Liquid phase $C_{p}^{\mu} = C_{p}^{\mu} = C_{p}^{\mu}$	H)(C _B) ₂) + (corr-(F)(F) Literatur	(4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48 193.72	2.78 -1.51	Reference 78HAR/HEA 73AND/MAR	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1-\text{Fluoro-3-}}{(1 \times \text{C-}(C))}$ Gas phase $\Delta_t H^{\circ} = \frac{1}{2} \frac{1}{2}$	257.32 (trifluorome H)(C_B) ₂) + (1	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _E × meta corr-(F) e - Calculated	-17.18 -17.18 -17.18 -17.18 -17.18 -17.18	73AND/MAR C7H4F C)(C _B) ₂) +
$(2 \times C_B - (F + F)^2)$ $(2 \times meta + G + F)$ $(2 \times meta + G + F)$ $C_P^o = C_P^o = C_P^o = C_P^o = S_P^o = S_$	H)(C _B) ₂) + (corr-(F)(F) Literatur	(4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48 193.72 274.50	= Residual	Reference 78HAR/HEA	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1-\text{Fluoro-3-}(4 \times C_B - C)}{(1 \times C - C)}$	257.32 (trifluorome H)(C_B) ₂) + (1 C_B) ₃) + (1	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _E × meta corr-(F)	-17.18 $(a)_{2} + (1 \times C_{B} - (CF3))$ = Residual	73AND/MAR C_7H_4F $C)(C_B)_2) +$ Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ $C_p^\circ = S^\circ = \Delta_t S^\circ =$	H)(C _B) ₂) + (corr-(F)(F) Literatur	(4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48 193.72 274.50 -295.88	2.78 -1.51	Reference 78HAR/HEA 73AND/MAR	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = \frac{1-\text{Fluoro-3-}}{(1 \times \text{C-}(C))}$ Gas phase $\Delta_t H^{\circ} = \frac{1}{2} \frac{1}{2}$	257.32 (trifluorome H)(C_B) ₂) + (1 C_B) ₃) + (1	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _E × meta corr-(F) e - Calculated	-17.18 $(a)_{2} + (1 \times C_{B} - (CF3))$ = Residual	73AND/MAR C_7H_4F $C)(C_B)_2) +$ Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ =$	H)(C _B) ₂) + (corr-(F)(F) Literatur	(4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48 193.72 274.50 -295.88 -598.26	2.78 -1.51	Reference 78HAR/HEA 73AND/MAR	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = 1$ 1-Fluoro-3-(4×C _B -((1×C-(C))) Gas phase $\Delta_t H^{\circ} = C_p^{\circ} = \frac{1}{2}$	257.32 (trifluorome H)(C _B) ₂) + (1 B)(F) ₃) + (1 Literatur - 792.20	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _E × meta corr-(F) e - Calculated	-17.18 $(a)_{2} + (1 \times C_{B} - (CF3))$ = Residual	73AND/MAR C_7H_4F $C)(C_B)_2) +$ Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ $C_p^\circ = S^\circ = \Delta_t S^\circ =$	H)(C _B) ₂) + (corr-(F)(F) Literatur	(4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48 193.72 274.50 -295.88	2.78 -1.51	Reference 78HAR/HEA 73AND/MAR	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t S^{\circ} = \ln K_t = 1$ 1-Fluoro-3-(4×C _B -(C)) Gas phase $\Delta_t H^{\circ} = C_p^{\circ} = 1$ Liquid phas	257.32 (trifluorome H)(C _B) ₂) + (1 B)(F) ₃) + (1 Literatur - 792.20	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _E × meta corr-(F) e - Calculated	-17.18 $(a)_{2} + (1 \times C_{B} - (CF3))$ = Residual	73AND/MAR C_7H_4F $C)(C_B)_2) +$ Reference
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} =$ $\Delta_{t}G^{\circ} =$	H)(C _B) ₂) + (corr-(F)(F) Literatur	(4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48 193.72 274.50 -295.88 -598.26	2.78 -1.51	Reference 78HAR/HEA 73AND/MAR	$C_{\rho}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \ln K_{t} = \frac{1 - \text{Fluoro-} 3 - (4 \times C_{B} - C)}{(1 \times C - C)}$ Gas phase $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = \frac{1 - \text{Fluoro-} 3 - (4 \times C_{B} - C)}{(1 \times C - C)}$ Liquid phas	257.32 (trifluorome H)(C _B) ₂) + (1 B)(F) ₃) + (1 Literatur - 792.20	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _B × meta corr-(F) e - Calculated - 792.17 142.59	- 17.18 (a) ₂) + (1 × C _B -(F)(CF3)) = Residual - 0.03	73AND/MAR C ₇ H ₄ F C)(C _B) ₂) + Reference 59GOO/DOU
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $\Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} =$ $\ln K_{t} =$	H)(C _B) ₂) + (corr-(F)(F) Literatur - 683.70 192.21 250.41	(4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48 193.72 274.50 -295.88 -598.26 241.34	2.78 -1.51	78HAR/HEA 73AND/MAR	$C_{\rho}^{\circ} = S^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = \ln K_{t} = \frac{1 - \text{Fluoro-} 3 - (4 \times C_{B} - C)}{(1 \times C - C)}$ Gas phase $\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = \frac{1 - \text{Fluoro-} 3 - (4 \times C_{B} - C)}{(1 \times C - C)}$ Liquid phas	257.32 (trifluorome H)(C _B) ₂) + (1 B)(F) ₃) + (1 Literatur - 792.20	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _B × meta corr-(F) e - Calculated - 792.17 142.59	- 17.18 (a) ₂) + (1 × C _B -(F)(CF3)) = Residual - 0.03	73AND/MAR C7H4F C)(CB)2) + Reference 59GOO/DOU
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $C_{p}^{\circ} = G_{p}^{\circ} =$ $\Delta_{t}G^{\circ} = G_{p}^{\circ} =$ $\ln K_{t} =$ 1,2,3,4-Tetra	H)(C _B) ₂) + (corr-(F)(F) Literatur - 683.70 192.21 250.41	(4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48 193.72 274.50 -295.88 -598.26 241.34	2.78 -1.51 -24.09	78HAR/HEA 73AND/MAR 73AND/MAR	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = 1$ 1-Fluoro-3-(4×C _B -(1) (1×C-(C) Gas phase $\Delta_t H^{\circ} = C_p^{\circ} = 1$ Liquid phas $\Delta_t H^{\circ} = 1$	(trifluorome H)(C _B) ₂) + (1 E)(F) ₃) + (1 Literatur - 792.20	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _B × meta corr-(F) e - Calculated - 792.17 142.59	- 17.18 (a) ₂) + (1 × C _B -(F)(CF3)) = Residual - 0.03	73AND/MAR C ₇ H ₄ F C)(C _B) ₂) + Reference 59GOO/DOU
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t G^\circ = C_p^\circ = C_p^\circ =$ $\Delta_t G^\circ = C_p^\circ = C_p^\circ =$ $1,2,3,4\text{-Tetra}$	H)(C _B) ₂) + (corr-(F)(F) Literatur - 683.70 192.21 250.41	(4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48 193.72 274.50 -295.88 -598.26 241.34	2.78 -1.51 -24.09	78HAR/HEA 73AND/MAR 73AND/MAR	$C_p^{\circ} = S^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t = 1$ 1-Fluoro-3-($(4 \times C_B - C_t)$) (1 \times C - C_t) Gas phase $\Delta_t H^{\circ} = C_p^{\circ} = 1$ Liquid phas $\Delta_t H^{\circ} = 1$	(trifluorome H)(C _B) ₂) + (1 E _B)(F) ₃) + (1 Literatur - 792.20 e - 830.20	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _E × meta corr-(F) e - Calculated - 792.17 142.59 - 830.06	- 17.18 (a) ₂) + (1 × C _B -(F)(CF3)) = Residual - 0.03	73AND/MAR C7H4F C)(CB)2) + Reference 59GOO/DOU C6HF2
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t G^\circ = C_p^\circ = C_p^\circ =$ $\Delta_t G^\circ = C_p^\circ = C_p^\circ =$ $1,2,3,4\text{-Tetra}$	H)(C _B) ₂) + (corr-(F)(F) Literatur -683.70 192.21 250.41 fluorobenz H)(C _B) ₂) + ((4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48 193.72 274.50 -295.88 -598.26 241.34	2.78 -1.51 -24.09	78HAR/HEA 73AND/MAR 73AND/MAR	$C_p^\circ = S^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1 - \text{Fluoro-} 3 - (4 \times C_B - (1 \times C - (C)))}{(1 \times C - (C))}$ Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{1 - (C + C)}{(1 \times C_B - (1 \times C_B - (C)))}$ Pentafluoroi $(1 \times C_B - (C + C))$	(trifluorome H)(C _B) ₂) + (1 E _B)(F) ₃) + (1 Literatur - 792.20 e - 830.20	274.50 - 295.88 - 598.26 241.34 ethyl) benzene (1 × C _B -(F)(C _E × meta corr-(F) e - Calculated - 792.17 142.59 - 830.06	- 17.18 (a) ₂) + (1 × C _B -(F)(CF3)) = Residual - 0.03	73AND/MAR C ₇ H ₄ F C)(C _B) ₂) + Reference 59GOO/DOU
Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ $\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$ $\ln K_t =$ 1,2,3,4-Tetra $(2 \times C_B - (1 + 1)^2)$	H)(C _B) ₂) + (corr-(F)(F) Literatur -683.70 192.21 250.41 fluorobenz H)(C _B) ₂) + ((4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48 193.72 274.50 -295.88 -598.26 241.34 ene (4×C _B -(F)(C _B)	2.78 -1.51 -24.09	78HAR/HEA 73AND/MAR 73AND/MAR C ₆ H ₂ F ₄	$C_p^\circ = S^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1 - \text{Fluoro-} 3 - (4 \times C_B - (1 \times C - (C)))}{(1 \times C - (C))}$ Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{1 - (C + C)}{(1 \times C_B - (1 \times C_B - (C)))}$ Pentafluoroi $(1 \times C_B - (C + C))$	(trifluorome H)(C _B) ₂) + (1 Literatur - 792.20 e - 830.20 benzene H)(C _B) ₂) + (1 corr-(F)(F)	274.50 - 295.88 - 598.26 241.34 ethyl) benzene (1 × C _B -(F)(C _E × meta corr-(F) e - Calculated - 792.17 142.59 - 830.06	-17.18 $-$	73AND/MAR C7H4F C)(CB)2) + Reference 59GOO/DOU C6HF
Gas phase $\Delta_t H^\circ = C_p^\circ = $ Liquid phase $\Delta_t H^\circ = C_p^\circ = $ $\Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = $ $\ln K_t = $ 1,2,3,4-Tetra (2 × C _B -(F	H)(C _B) ₂) + (corr-(F)(F) Literatur -683.70 192.21 250.41 fluorobenz H)(C _B) ₂) + ((4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48 193.72 274.50 -295.88 -598.26 241.34 ene (4×C _B -(F)(C _B)	2.78 -1.51 -24.09	78HAR/HEA 73AND/MAR 73AND/MAR C ₆ H ₂ F ₄	$C_p^\circ = S^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1 - \text{Fluoro-} 3 - (4 \times C_B - (1 \times C - (C)))}{(1 \times C - (C))}$ Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{1 - (C + C)}{(1 \times C_B - (1 \times C_B - (C)))}$ Pentafluoroi $(1 \times C_B - (C + C))$	(trifluorome H)(C _B) ₂) + (1 Literatur - 792.20 e - 830.20 benzene H)(C _B) ₂) + (1 corr-(F)(F)	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _B × meta corr-(F) e - Calculated - 792.17 142.59 - 830.06	-17.18 $-$	73AND/MAR C7H4F C)(CB)2) + Reference 59GOO/DOU 59GOO/DOU C4HF corr-(F)(F)) +
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} =$ 1,2,3,4-Tetra $(2 \times C_{B} - (H^{\circ}))$ Gas phase	H)(C _B) ₂) + (corr-(F)(F) Literatur -683.70 192.21 250.41 fluorobenz H)(C _B) ₂) + ((4×C _B -(F)(C _B)) e - Calculated = -655.62 131.62 -686.48 193.72 274.50 -295.88 -598.26 241.34 ene (4×C _B -(F)(C _B)	2.78 -1.51 -24.09	78HAR/HEA 73AND/MAR 73AND/MAR C ₆ H ₂ F ₄	$C_p^\circ = S^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1 - \text{Fluoro-} 3 - (4 \times C_B - (1 \times C - (C)))}{(1 \times C - (C))}$ Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{1 - (C + C)}{(1 \times C_B - (1 \times C_B - (C)))}$ Pentafluoroi $(1 \times C_B - (C + C))$	(trifluorome H)(C _B) ₂) + (1 Literatur - 792.20 e - 830.20 benzene H)(C _B) ₂) + (1 corr-(F)(F)	274.50 - 295.88 - 598.26 241.34 ethyl)benzene (1 × C _B -(F)(C _B × meta corr-(F) e - Calculated - 792.17 142.59 - 830.06	-17.18 $-$	73AND/MAR C7H4F C)(CB)2) + Reference 59GOO/DOU 59GOO/DOU C4HF corr-(F)(F)) +

TABLE	50.	Fluorides	(46)	–	Continued
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Pentafluorobenzene (Continued) $(1 \times C_B-(H)(C_B)_2) + (5 \times C_B-(F)(C_B)_2) + (4 \times ortho \ c$ $(1 \times meta \ corr-(F)(F))$	C_6HF_5 orr- $(F)(F)$ +	Acetyl fluoride $(1 \times C - (H)_3(CO)) + (1 \times CO - (C)(F))$
Literature - Calculated = Residual	Reference	Literature – Calculated – Residual Reference
Liquid phase $\Delta_0 H^\circ = -841.80 - 841.84 0.04$	69COX/GUN	Gas phase $\Delta_t H^o = -422.10 -422.10$ 0.00 70COX/PIL
$C_{\rho}^{\circ} = 204.68$ 208.13 -3.45 $S^{\circ} = 275.89$ 299.82 -23.93 $\Delta_{\epsilon}S^{\circ} = -306.61$ $\Delta_{f}G^{\circ} = -750.42$ $\ln K_{f} = 302.72$	68COU/HAL 68COU/HAL	Liquid phase $\Delta_t H^\circ = -467.20 -467.20 0.00 49CAR/SKI$
2,3,4,5,6-Pentafluorotoluene	C7H3F5	2,2,2-Trifluoroethanol $(1 \times C - (C)(F)_3) + (1 \times C - (H)_2(O)(C)) + (1 \times O - (H)(C))$ Literature Coloulated - Residuel
$(1 \times C_{-}(H)_{3}(C)) + (1 \times C_{B-}(C)(C_{B})_{2}) + (5 \times C_{B-}(F)(C_{B})_{2}) + (5 \times C_{B-}(F)(C_{B})_{2}) + (2 \times ortho \ corr-(alk)(X))$	-BJ2J +	Literature - Calculated = Residual Reference
Literature – Calculated = Residual	Reference	Gas phase $\Delta_t H^\circ = -888.40 -866.04 -22.36$ 73ROC/SYM $C_b^\circ = 91.48$
Gas phase $\Delta_l H^\circ = -842.90 - 836.30 - 6.60$ $C_\rho^\circ = 165.98$	69COX/GUN	Liquid phase
Liquid phase $ \Delta_{t}H^{\circ} = -883.80 -871.85 -11.95 $ $ C_{\rho}^{\circ} = 232.03 $ $ S^{\circ} = 334.75 $ $ \Delta_{t}S^{\circ} = -407.99 $ $ \Delta_{t}G^{\circ} = -750.21 $ $ \ln K_{t} = 302.63 $	69COX/GUN	$\Delta_t H^\circ = -932.40 -936.37$ 3.97 71KOL/IVA $C_p^\circ = 151.46$ $S^\circ = 212.04$ $\Delta_t S^\circ = -401.84$ $\Delta_t G^\circ = -816.56$ $\ln K_t = 329.40$
102.05		$\begin{array}{ll} \textbf{3,3,3-Trifluoro-1-propanol} & \textbf{C_3H_5F_3O} \\ (1\times O-(H)(C)) + (1\times C-(H)_2(O)(C)) + (1\times C-(H)_2(C)_2) + \\ (1\times C-(C)(F)_3) & \end{array}$
Dodecasiuorocyclohexane $(6 \times C - (C)_2(F)_2) + (1 \times Cyclohexane (sub) rsc)$	C ₆ F ₁₂	Literature - Calculated = Residual Reference
Literature - Calculated = Residual	Reference	Gas phase
Gas phase $\Delta_{\mu}H^{\circ} = -2370.40 -2468.73$ 98.33 $C_{\rho}^{\circ} = 225.70$	79PRI/SAP	$\Delta_l H^\circ = -886.67$ $C_p^\circ = 114.37$
Liquid phase $\Delta_t H^\circ = -2406.30 -2404.28 -2.02$	79PRI/SAP	Liquid phase $\Delta_t H^\circ = -969.60 -962.10 -7.50$ 69KOL/IVA $C_\rho^\circ = 181.88$ $S^\circ = 244.42$ $\Delta_t S^\circ = -505.77$
Solid phase $\Delta_t H^\circ = -2562.32$		$\Delta_{t}G^{\circ} = -811.30$ $\ln K_{t} = 327.27$

TABLE 50. Fluorides (46) - Continued

	+(1×C-(H	C ₃ H ₄ F ₄ I) ₂ (O)(C)) +	2,2,3,3,4,4,4-Heptafiuoro-1-butanol C_4H_3F (1×O-(H)(C))+(1×C-(H) ₂ (O)(C))+(2×C-(C) ₂ (F) ₂)+
(1×O-(H)(C))		<i>7</i> - <i>x 7x 7y</i>	$(1\times C-(C)(F)_3)$
Literature - Calculated =	Residual	Reference	Literature - Calculated = Residual Reference
Gas phase $\Delta_t H^\circ = -1061.30 -1058.36$ $C_p^\circ = 122.13$	- 2.94	73ROC/SYM	Gas phase $\Delta_t H^\circ = -1688.82$ $C_\rho^\circ = 174.32$
Liquid phase $\Delta_t H^{\circ} = -1114.90 -1114.90$	0.00	69KOL/IVA	Liquid phase $\Delta_t H^\circ = -1781.90 -1737.11 -44.79$ 71KOL/IVA2
2,2,3,3,3-Pentafluoro-1-propanol (1 × O-(H)(C)) + (1 × C-(H) ₂ (O)(C)) (1 × C-(C)(F) ₃)	+(1×C-(C	C₃H₃F₅O ()2(F)2) +	2,2,3,3,4,4,5,5-Octafluoro-1,6-hexanediol $(2 \times O - (H)(C)) + (2 \times C - (H)_2(O)(C)) + (4 \times C - (C)_2(F)_2)$
Literature – Calculated =	Residual	Reference	Literature – Calculated = Residual Reference
Gas phase $\Delta_t H^\circ = -1310.30 -1277.43$ $C_p^\circ = 132.90$	-32.87	73ROC/SYM	Gas phase $\Delta_t H^\circ = -2084.20 -2030.02 -54.18$ 74KOL/SLA $C_p^\circ = 242.66$
Liquid phase $\Delta_t H^\circ = -1354.70 -1336.74$	-17.96	69KOL/IVA	Liquid phase $\Delta_t H^\circ = -2056.08$
			Solid phase
Pentafluorophenol $(1 \times O-(H)(C_B)) + (1 \times C_B-(O)(C_B)_2)$ $(4 \times ortho \text{ corr-}(F)(F))$	+ (5 × C _B -(I	C_6HF_5O F)(C _B) ₂)+	$\Delta_t H^\circ = -2173.40 - 2180.40$ 7.00 74KOL/SLA
			Pentafluorobenzoic acid C_7HF_5 ($(1 \times O-(H)(CO)) + (1 \times CO-(O)(C_B)) + (5 \times C_B-(F)(C_B)_2) + (4 \times ortho \ corr-(F)(F)) + (1 \times C_B-(CO)(C_B)_2) +$
$(1 \times O - (H)(C_B)) + (1 \times C_B - (O)(C_B)_2)$ $(4 \times ortho \text{ corr-}(F)(F))$ $Literature - Calculated =$ $Gas phase$ $\Delta_t H^\circ = -956.80 - 987.75$		F)(C _B) ₂)+	Pentafluorobenzoic acid C_7HF_5 $(1 \times O-(H)(CO)) + (1 \times CO-(O)(C_B)) + (5 \times C_B-(F)(C_B)_2) +$
$(1 \times O - (H)(C_B)) + (1 \times C_B - (O)(C_B)_2)$ $(4 \times ortho \text{ corr-}(F)(F))$ $Literature - Calculated =$ $\Delta_t H^\circ = -956.80 - 987.75$ $C_p^\circ = 164.52$ $Liquid phase$ $\Delta_t H^\circ = -1007.70 - 1053.36$	Residual	Reference	Pentafluorobenzoic acid C_7HF_5 ($(1 \times O-(H)(CO)) + (1 \times CO-(O)(C_B)) + (5 \times C_B-(F)(C_B)_2) + (4 \times ortho \ corr-(F)(F)) + (1 \times C_B-(CO)(C_B)_2) + (2 \times ortho \ corr-(F)(COOH))$
$(1 \times O-(H)(C_B)) + (1 \times C_B-(O)(C_B)_2)$ $(4 \times ortho \text{ corr-}(F)(F))$ $Literature - Calculated =$ $Gas phase$ $\Delta_t H^\circ = -956.80 -987.75$ $C_p^\circ = 164.52$ $Liquid phase$	Residual 30.95	F)(C _B) ₂) + Reference 69COX/GUN	Pentafluorobenzoic acid C_7HF_5 $(1 \times O - (H)(CO)) + (1 \times CO - (O)(C_B)) + (5 \times C_B - (F)(C_B)_2) + (4 \times ortho \text{ corr-}(F)(F)) + (1 \times C_B - (CO)(C_B)_2) + (2 \times ortho \text{ corr-}(F)(COOH))$ Literature – Calculated = Residual Reference

(1×CO-($F(C_B)_2 + (4 \times C_{B} - (H)(C_B)_2) + (1 \times C_{B} - (CO)(C_B)_2) + (1 \times C_{B} - (CO)($	C ₇ H ₅ FO ₂ O-(H)(CO)) +	4-Fluorobenzoic acid $(4 \times C_B-(H)(C_B)_2) + (1 \times CO-(O)(C_B)) + (1 \times CO-(O)(C_B))$	$(1 \times C_B - (F)(C_B)_2$		С 7HsF0 ; H)(CO))+
(1×onno	corr-(F)(COOH)) Literature – Calculated = Residual	Reference	Literatu	re – Calculated =	Residual	Reference
			Solid phase			
Gas phase $\Delta_t H^\circ =$	469.82		$ \Delta_t H^\circ = -568.60 $ $ C_p^\circ = S^\circ = $	-586.88 158.03 184.78	18.28	56SCO/GOO
			$\Delta_{f}S^{\circ} =$	- 488.21		
Liquid phase $\Delta_t H^\circ =$	e 573.70		$\Delta_t G^{\circ} = \ln K_t =$	- 441.32 178.03		
$C_p^{\circ} =$	218.18			176.03		
Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	- 567.60 - 566.88 - 0.72 158.03 184.78	56SCO/GOO	Bis-(3,3,3-trifluoropro (2 × C-(C)(F) ₃) + (2 (1 × O-(C) ₂)		(2×C-(H)₂(C ₆ H ₈ F ₆ O (O)(C))+
$\Delta_{\mathbf{f}}S^{\circ} =$	-488.21		Literatu	re - Calculated =	Residual	Reference
$\Delta_i G^{\circ} =$	-421.32					
lnK _f =	169.96		Gas phase $\Delta_l H^\circ = -1604.30$ $C_p^\circ =$	- 1556.10 210.96	-48.20	74SLA/KOL
3-Fluoroben		C ₇ H ₅ FO ₂				
	$H_1(C_B)_2 + (1 \times C_{B^{-1}}(F)(C_B)_2) + (1 \times C_{B^{-1}}(F)(C_B)_2)$ $H_1(C_B)_2 + (1 \times C_{B^{-1}}(CO)(C_B)_2)$)-(H)(CO))+	Liquid phase			
(1207	Literature – Calculated = Residual	Reference	$\Delta_t H^\circ = -1645.30$ $C_\rho^\circ =$	- 1652.03 298.75	6.73	74SLA/KOL
			$S^{\circ} = \Delta_{\epsilon}S^{\circ} =$	427.84 839.45		
Gas phase $\Delta_t H^\circ =$	- 489.82		$\Delta_f G^\circ = \\ \ln K_f =$	- 1401.75 565.46		
Liquid phas				_		
$\Delta_t H^\circ = C_r^\circ =$	- 573.70 218.18		Octafluoropropane; Po $(2 \times C - (C)(F)_3) + (1$			C ₃ F ₈
Solid phase			Literatu	re – Calculated = 1	Residual	Reference
$C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = 0$	- 582.00 - 586.88 4.88 158.03 184.78 - 488.21	56SCO/GOO	Gas phase $\Delta_t H^\circ = -1760.12$ $C_p^\circ =$	1759.01 147.40	-1.11	67KOL/TAL
$\Delta_f G^\circ = \ln K_f =$	-441.32 178.03					
	zoic acid H)(C_B) ₂) + (1 × C_B -(F)(C_B) ₂) + (1 × C_B -(CO)(C_B) ₂) Literature – Calculated = Residual					
Gas phase Δ _i H° =	494.50 489.82 4.68	69COX/GUN				
Liquid phas $\Delta_t H^\circ =$	-573.70					
$C_p^{\circ} =$	218.18					

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	T	ABLE 51. Chlo	rides (116)			TABLE 5	1. Chlorides (116) — Conti	inued
	nane; Methy H) ₃ (Cl), met	l chloride hyl chloride), c	$\sigma = 3$	CH₃Cl	1-Chlorobu (1×C-(1		× C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂	C_4H_9C (C)(Cl)), $\sigma = 3$
	Literatur	e – Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase					Gas phase				
$\Delta_t H^{\circ} =$	~81.90	-81.90	0.00	71FLE/PIL	$\Delta_{\epsilon}H^{\circ} =$	-154.60	-152.97	-1.63	68WAD
$C_p^{\circ} =$	40.75	40.75	0.00	69STU/WES	$C_p^{\circ} =$	107.57	109.04	-1.47	69STU/WES
S° =	234.37	234.47	-0.10	69STU/WES	S° =	358.07	355.75	2.32	69STU/WES
$\Delta_f S^\circ =$		-78.62			$\Delta_{\mathbf{f}}S^{\circ} =$		-366.27		
$\Delta_{\rm f}G^{\circ} =$		- 58.46			$\Delta_t G^\circ =$		-43.77		
$lnK_f =$		23.58		<u> </u>	$lnK_f =$		17.66	·	- · · · · · · · · · · · · · · · · · · ·
					Liquid pha				
Chloroetha				C ₂ H ₅ Cl	$\Delta_{\rm f}H^{\circ} =$	- 188.10	- 185.97	-2.13	75STR/SUN
(1 × C-(1	H) ₃ (C)) + (1	\times C-(H) ₂ (C)(C	(1)), $\sigma = 3$		$C_p^{\circ} =$	159.64	161.08	- 1.44	85LAI/WIL
	7.	0.1.1.1	D	D. f.	S° =		252.33		
	Literatur	e – Calculated	= Kesidual	Reference	$\Delta_f S^\circ =$	*	-469.69		
					$\Delta_{\rm f}G^{\circ} =$		-45.93		
Gas phase					$lnK_f =$		18.53		
$\Delta_t H^\circ =$	- 112.26	- 111.71	-0.55	71FLE/PIL					
$C_p^{\circ} =$	62.72	63.26	-0.54	69STU/WES	1-Chlorope	entane			C ₅ H ₁₁ C
S° =	275.85	277.43	-1.58	69STU/WES	(1×C-(I	$H)_3(C)) + (3$	\times C-(H) ₂ (C) ₂)	$+(1\times C-(H)_2)$	$(C)(Cl)), \sigma = 3$
$\Delta_f S^\circ =$		- 171.97							
$\Delta_{\mathbf{f}}G^{\circ} =$		- 60.44				Literatu	re – Calculated	= Residual	Reference
$lnK_f =$		24.38						·	
					Gas phase				
Liquid pha	is e				$\Delta_{\mathbf{f}}H^{\circ}$ –	-175.20	-173.60	-1.60	68WAD
$\Delta_{\rm f}H^{\circ} =$	- 136.90	- 134.51	-2.39	48GOR/GIA	$C_p^{\circ} =$	130.46	131.93	-1.47	69STU/WES
$C_p^{\circ} =$	103.30	100.24	3.06	48GOR/GIA	S° =	397.02	394.91	2.11	69STU/WES
S° =	186.27	187.57	-1.30	48GOR/GIA	$\Delta_f S^\circ =$		-463.42		
$\Delta_f S^\circ =$		-261.82			$\Delta_{\rm f}G^{\circ} =$		-35.43		
$\Delta_f G^\circ = \ln K_f =$		- 56.45 22.77			$lnK_f =$		14.29	. <u></u>	
				·	Liquid pha	50			
					$\Delta_f H^\circ =$	- 213.44	-211.70	- 1.74	75STR/SUN
1-Chloropi	ropane			C ₃ H ₇ Cl	$C_p^{\circ} =$		191.50		
•	•	\times C-(H) ₂ (C) ₂)	$+(1\times C-(H)_2$	$(C)(CI)), \sigma = 3$	S° =		284.71		
` `	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	. , , , , , , ,	` ` ` ?-		$\Delta_{\mathbf{f}}S^{\circ} =$		-573.62		
	Literatu	re – Calculated	= Residual	Reference	$\Delta_f G^\circ =$		-40.68		
					$lnK_f =$		16.41		
Gas phase									* .
$\Delta_{\rm f}H^{\circ} =$	-132.51	-132.34	-0.17	71FLE/PIL	1-Chlorooc	tane			C ₈ H ₁₇ C
$C_p^{\circ} =$	84.68	86.15	- 1.47	69STU/WES	(1×C-(I	$H)_3(C)) + (6$	\times C-(H) ₂ (C) ₂)	$+(1\times C-(H)_{2})$	(C)(Cl))
S° =	319.11	316.59	2.52	69STU/WES					_ 1
$\Delta_f S^{\circ} -$		- 269.12				Literatur	c – Calculated	- Residual	Reference
$\Delta_f G^\circ =$		-52.10							
$lnK_f =$		21.02			Gos phose				
					Gas phase $\Delta_t H^\circ =$	-238.88	-235.49	-3.39	68WAD
Liquid pha	ase				$C_p^{\circ} =$	20.00	200.60	3.33	, WHAD
$\Delta_i H^\circ =$	~ 160.40	-160.24	-0.16	77MAN/SEL	О р			-	
$C_p^{\circ} =$	131.38	130.66	0.72	1881REI					
S° =		219.95	· -	· · · · · · · · · · · · · · · · · · ·	Liquid pha	se			
		-365.75			$\Delta_i H^\circ =$	-291.30	-288.89	-2.41	75STR/SUN
$\Delta_{\mathbf{f}}S^{\circ} =$		-51.19			$C_p^{\circ} =$		282.76		
							201.05		
$\Delta_f S^\circ =$		20.65			S° =		381.85		
$\Delta_f S^\circ = \Delta_f G^\circ =$		20.65			$\Delta_{\mathbf{f}}S^{\circ} =$		-885.41		
$\Delta_f S^\circ = \Delta_f G^\circ =$		20.65							

TABLE 51.	Chlorides ((116) -	Continued
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TABLE 51. Chlorides (116) - Continued

1-Chlorododecane $(1 \times C - (H)_3(C)) + (10 \times C - (H)_2(C)_2) + (1 \times$	C ₁₂ H ₂₅ Cl	1-Chloro-2-methylpropane C_4H_5C $(2\times C-(H)_3(C))+(1\times C-(H)(C)_3)+(2\times -CH_3 \text{ corr (tertiary)})+$ $(1\times C-(H)_2(C)(Cl)), \sigma=9$
Literature – Calculated = Residual	Reference	$Literature - Calculated = Residual \qquad Reference$
Gas phase $\Delta_t H^\circ = -321.98 -318.01 -3.97$ $C_p^\circ = 292.16$ Liquid phase $\Delta_t H^\circ = -392.31 -391.81 -0.50$	75STR/SUN	Gas phase $\Delta_t H^\circ = -159.40 -159.66 0.26 68WAD$ $C_p^\circ = 108.49 109.07 -0.58 69STU/WES$ $S^\circ = 353.80 342.01 11.79 69STU/WES$ $\Delta_t S^\circ = -380.00$ $\Delta_t G^\circ = -46.36$
$C_p^{\circ} = 404.44$ $S^{\circ} = 511.37$ $\Delta_t S^{\circ} = -1301.13$ $\Delta_t G^{\circ} = -3.88$ $\ln K_t = 1.56$		$\ln K_{\rm f} = 18.70$ Liquid phase $\Delta_{\rm f} H^{\circ} = -191.10 -191.25$ 0.15 53SMI/BJE $C_{\rm p}^{\circ} = 158.57$ 158.10 0.47 48KUR
1-Chlorooctadecane $(1 \times C-(H)_3(C)) + (16 \times C-(H)_2(C)_2) + (1 \times C-(H)_2(C)_2)$		$S^{\circ} = 246.98$ $\Delta_{f}S^{\circ} = -475.04$ $\Delta_{f}G^{\circ} = -49.62$ $\ln K_{f} = 20.02$
Literature – Calculated = Residual Gas phase	Reference	2-Chloropropane C_3H_7C (2×C-(H) ₃ (C)) + (1×C-(H)(C) ₂ (Cl)) +
$\Delta_t H^{\circ} = -446.04 -441.79 -4.25$ $C_p^{\circ} = 429.50$	75STR/SUN	(2×-CH ₃ corr (tertiary)), σ = 9 Literature – Calculated = Residual Reference
Liquid phase $\Delta_{t}H^{\circ} = -544.20 \qquad -546.19 \qquad 1.99$ $C^{\circ}_{\rho} = \qquad 586.96$ $S^{\circ} = \qquad 705.65$ $\Delta_{t}S^{\circ} = \qquad -1924.72$ $\Delta_{t}G^{\circ} = \qquad 27.67$ $\ln K_{t} = \qquad -11.16$	75STR/SUN	Gas phase $ \Delta_t H^\circ = -144.90 \qquad -144.65 \qquad -0.25 \qquad 71 \text{FLE/PIL} $ $ C_p^\circ = 87.32 \qquad 86.46 \qquad 0.86 \qquad 69 \text{STU/WES} $ $ S^\circ = 304.18 \qquad 307.71 \qquad -3.53 \qquad 69 \text{STU/WES} $ $ \Delta_t S^\circ = \qquad -277.99 \qquad $
1-Chloro-3-methylbutane $(2\times C-(H)_3(C)) + (1\times C-(H)_2(C)_2) + (1\times C-(H)(C)_2(C)_2) + (1\times C-(H)(C)_2(C)(C)_2), \ \sigma$ (2×-CH ₃ corr (tertiary)) + (1×C-(H) ₂ (C)(Cl)), \ \sigma		Liquid phase $\Delta_c H^{\circ} = -172.10 -170.75 -1.35$ 31MAT/FEH $C_p^{\circ} = 138.98$
Literature - Calculated = Residual	Reference	2-Chlorobutane C ₄ H ₂ C
Gas phase $\Delta_l H^\circ = -180.33 - 180.29 -0.04$ $C_p^\circ = 133.89 131.96 1.93$ $S^\circ = 399.82 381.17 18.65$ $\Delta_l S^\circ = -477.16$	69STU/WES 69STU/WES 69STU/WES	$(2 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)_2(Cl)), \sigma = 9$ Literature – Calculated = Residual Reference
$\Delta_{i}G^{\circ} = -38.03$ $\ln K_{\rm f} = 15.34$ Liquid phase $\Delta_{i}H^{\circ} = -216.98 -216.98 0.00$ $C_{\rho}^{\circ} = 179.50 188.52 -9.02$	69STU/WES 48KUR	Gas phase $\Delta_t H^\circ = -161.20 - 160.76 - 0.44$ 68WAD $C_p^\circ = 108.49$ 109.35 -0.86 69STU/WES $S^\circ = 350.41$ 346.87 3.54 69STU/WES $\Delta_t S^\circ = -375.14$ $\Delta_t G^\circ = -48.91$ $\ln K_t = 19.73$
$S^{\circ} = 279.36$ $\Delta_t S^{\circ} = -578.97$ $\Delta_t G^{\circ} = -44.36$ $\ln K_t = 17.89$		Liquid phase $\Delta_{\rho}H^{\circ} = -192.80 - 192.12 - 0.68$ 53SMI/BJE $C_{\rho}^{\circ} = 169.40$

TABLE 51. Chlorides (116) - Continued

TABLE 51. Chlorides (116) - Continued

2-Chlorohex (2×C-(H		\times C-(H) ₂ (C) ₂)	- (1×C-(H)($C_6H_{13}CI$ $C)_2(CI))$	$(3 \times C - (1 \times C - (1 \times C + C)))$		nne × C-(H)2(C)2) ternary)) + (1 ×		$C_sH_{ii}C$ $\sigma = 27$
	Literatur	e – Calculated =	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 203.30	-202.02 155.13	-1.28	68WAD	Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 202.20 131.59	- 200.23 129.71	-1.97 1.88	31MAT/FEH 69STU/WES
Liquid phas $\Delta_t H^\circ = C_p^\circ =$	e 246.10	- 243.58 230.24	- 2.52	56KIR	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$	368,44	369.46 - 488.87 - 54.47 21.97	-1.02	69STU/WES
		ne × C-(H)(C) ₃) +	(2×−CH ₃ co	C5H11Cl orr (tertiary))+	Liquid pha $\Delta_t H^\circ =$	ese - 235.70	-234.12	-1.58	53SMI/BJE
	Literatui	e – Calculated	= Residual	Reference	1,2-Dichlor (2×C-(1	oethane H) ₂ (C)(Cl))	$\sigma = 2$		C₂H₄C
Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 185.10	- 188.08 132.27	2.98	68WAD		Literatu	re – Calculated	= Residual	Reference
Liquid phase $\Delta_t H^\circ = C_r^\circ =$	se 226.60	- 223.13 196.84	-3.47	73ESI/KAB	Gas phase $ \Delta_{f}H^{\circ} = \\ C_{p}^{\circ} = \\ S^{\circ} = \\ \Delta_{f}S^{\circ} = \\ \Delta_{f}G^{\circ} = \\ \ln K_{f} = $	-129.10 78.66 308.19	-138.90 75.06 312.72 -182.88 -84.38 34.04	9.80 3.60 - 4.53	58SIN/STU 69STU/WES 69STU/WES
(3×C-(I	C) ₃ (Cl)), σ	×-CH ₃ corr (q	•	C₄H₃Cl Reference	Liquid pha $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = $	se - 164.50 128.87 208.53	-173.80 127.52 208.54 -287.05 -88.21	9.30 1.35 - 0.01	58SIN/STU 40PIT 40PIT
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t = 1$	- 182.40 114.22 322.17	- 184.16 106.82 321.16 400.85 64.65 26.08	1.76 7.40 1.01	64LEV/AND 69STU/WES 69STU/WES			35.59 + (1×C-(H) ₃ (0, σ = 3	C))+	C₃H₅Cl
Liquid pha	se					Literatu	re – Calculated	= Residual	Reference
$\Delta_t H^{\circ} =$		- 212.78	1.38	68WAD	Gas phase $\Delta_t H^\circ =$ $C_\rho^\circ -$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	- 162.80 98.20 351.46	- 167.32 98.26 348.77 - 283.14 - 82.90 33.44	4.52 - 0.06 2.69	49DRE/MAR 69STU/WES 69STU/WES
					Liquid pha	se - 198.80	-205.68 166.26	6.88	49DRE/MAR

 $C_p^{\circ} =$

166.26

TABLE 51. Chlorides (116) - Continued

Table 51. Chlorides (116) - Continued

, 3-Dichlor (1×C–(H	opropane I) ₂ (C) ₂) + (2	×C~(H)2(C)(C	CI)), $\sigma = 2$	C₃H₅Ĉl₂		l)₃(C))+(1	Continued) \times C-(C) ₂ (Cl) ₂) ternary)), $\sigma \approx$		C₃H₄C
	Literatur	e – Calculated :	= Residual	Reference	Literature - Calculated = Residual			Reference	
C _p ° = S° = Δ _p S° =	- 159.20 99.62 351.08	-159,53 97,95 351,88 -280,03	0.33 1.67 -0.80	68WAD 69STU/WES 69STU/WES	Liquid phas $\Delta_t H^\circ = C_t^\circ =$	e 205.80	- 205.80 147.20	0.00	53SMI/BJE
$\Delta_t G^\circ = \ln K_t =$	· · · · · · · · · · · · · · · · · · ·	- 76.04 30.67			1,1,1-Trichle				C₂H₃C
Liquid phas	Se				(1×C-(H	l)₃(C))+(1	× C-(C)(Cl) ₃)		
$\Delta_t H^\circ = C_p^\circ = S^\circ =$	- 200.00	-199.53 157.94 240.92	-0.47	53SMI/BJE		Literatur	e – Calculated	= Residual	Reference
$\Delta_i S^\circ = \Delta_i G^\circ = \ln K_i =$		-390.98 -82.96 33.46			Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 145.00	- 124.24 93.91	- 20.76	71MAN/RIN
1,1-Dichlor (1 × C-(I		× C-(H)(C)(C	$(i)_2), \sigma = 3$	C ₂ H ₄ Cl ₂	Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = $	e 174.50 144.39 226.69	160.54 138.68 229.21	-13.96 5.71 -2.52	71MAN/RIN 73AND/COU 73AND/COU
	Literatui	re - Calculated	= Residual	Reference	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$		-312.58 -67.34 27.17		
Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	-127.60 76.23 304.97	- 121.36 76.42 301.47 - 194.13 - 63.48 25.61	-6.24 -0.19 3.50	67LAC/AMA 69STU/WES 69STU/WES	1,1,2-Trichle	I)(C)(Cl) ₂)	+ (1 × C-(H) ₂ (e		C₂H₃Cl Reference
Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	se 158.40 126.27 211.75	- 150.21 121.50 211.75 - 283.84 - 65.58 26.46	-8.19 4.77 0.00	56LI/PIT 56LI/PIT 56LI/PIT	Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = S^\circ = S$	- 151.20 88.99 337.10	-148.55 88.22 342.52 -199.27 -89.14 35.96	-2.65 0.77 -5.42	72LAY/WAD 69STU/WES 69STU/WES
	H)3(C))+(1 I3 corr (qua	$\times C - (C)_2(Cl)_2$ ternary)), $\sigma =$	18	C ₃ H ₆ Cl ₂	$C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} =$	e 191.50	- 189.50 148.78 232.72 - 309.07	-2.00	56KIR
Gas phase	Literatu	re – Calculated	= Kesidual	Reference	$\Delta_t G^\circ = \ln K_t =$		-97.35 39.27		
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	105.86 326.02	-173.20 105.86 326.02 -305.89 -82.00 33.08	0.00 0.00	69STU/WES 69STU/WES					

TABLE 51. Chlorides (116) — Continued

TABLE 51. Chlorides (116) - Continued

(= : :)	12(C)(CI))+	· (1×C-(H)(C)	$_2(Cl)), \sigma = 2$		(1×C-(H	$H_{2}(C)_{2}+($	$1 \times C - (C)(CI)_3$	$+(1\times C-(H)_2$	(C)(Cl))
	Literatur	e – Calculated	= Residual	Reference	Literature – Calculated – Residual		- Residual	Reference	
Gas phase					Gas phase		480.00		
$\Delta_{f}H^{\circ} = C_{p}^{\circ} =$	112.21	- 194.51 110.06	2.15	69STU/WES	$\Delta_t H^\circ = C_p^\circ =$		- 172.06 128.60		
$S^{\circ} =$	382.92	384.06	- 1.14	69STU/WES					
$\Delta_f S^\circ =$		-294.05							
$\Delta_t G^\circ = \ln K_t =$		- 106.84 43.10			Liquid pha $\Delta_t H^\circ =$	se 208.70	-225.56	16.86	70KOL/TOM
mrt –		45.10			$C_{\rho}^{\circ} =$	196.40	196.38	0.02	74KOL/VOR
					S° =	284.30	282.56	1.74	74KOL/VOR
Liquid phas		244.07	14.37	54BJE/SMI	$\Delta_{\mathbf{f}}S^{\circ} = \Delta_{\mathbf{f}}G^{\circ} =$		441.75 93.85		
$\Delta_t H^\circ = C_p^\circ =$	- 230.60 183.68	-244.97 193.54	- 9.86	41NEL/NEW	$\ln K_{\rm f} =$		- 93.85 37.86		
<i>p</i>									
	achloroeths			C ₂ H ₂ Cl ₄	Pentachlor (1×C-(0		i × C–(H)(C)(C	$(1)_2$), $\sigma = 3$	C ₂ HC
(2×C-(I	I)(C)(Cl) ₂),	$\sigma = 2$			Literature – Calculated = Residual		= Residual	Reference	
	Literatu	re – Calculated	= Residual	Reference	A				
G 1					Gas phase	142.00	161.00	10.00	ECVID.
Gas phase $\Delta_t H^\circ =$	- 148.80	- 158.20	9.40	72LAY/WAD	$\Delta_i H^{\circ} = C_{\rho}^{\circ} =$	- 142.00 117.74	- 161.08 118.87	19.08 1.13	56KIR 69STU/WES
$C_p^{\alpha} =$	100.79	101.38	-0.59	69STU/WES	S° =	380.53	376.29	4.24	69STU/WES
S° =	362.71	360.80	1.91	69STU/WES	$\Delta_f S^\circ =$		-257.91		
$\Delta_{\mathbf{f}}S^{\circ} =$		-227.20			$\Delta_t G^{\circ} =$		-84.18		
$\Delta_f G^\circ = \ln K_f =$		90.46 36.49			$lnK_f =$		33.96		
					Liquid pha	se			
Liquid pha					$\Delta_l H^{\circ} =$	- 189.90	-215.53	25.63	56KIR
$\Delta_i H^\circ =$	-194.60	- 205.20	10.60	53SMI/BJE	$C_p^{\circ} =$	196.23	187.22	9.01	48KUR
$C_{\rho}^{\circ} = S^{\circ} =$	165.27	170.04 256.90	-4.77	48KUR	$S^{\circ} = \Delta_{f}S^{\circ} =$		274.36 - 359.84		
$\Delta_f S^\circ =$		-331.10			$\Delta_{\rm f}G^{\circ} =$		- 108.25		
$\Delta_f G^\circ =$		- 106.48			$\ln K_{\rm f} =$		43.67		
$lnK_f =$		42.95	****			——————————————————————————————————————			
					Hexachloro (2×C-(0	ethane C)(Cl) ₃), σ	= 2		C₂Cl
	achloropro			C3H4Cl4	, ,				
(2×C-(1	H)₂(C)(Cl))	$+(1\times C-(C)_2(C)_2(C)_2(C)_2(C)_2(C)_2(C)_2(C)_2$	Cl) ₂)			Literatu	re – Calculated ––––	= Residual	Reference
	Literatu	re – Calculated	= Residual	Reference	Gas phase				
Gas phase					$\Delta_t H^{\circ} = C_{\rho} =$	- 143.50 136.36	- 163.96 136.36	20.46 0.00	63PUY/BAL 69STU/WES
Gas phase $\Delta_t H^\circ =$		- 218.46			$C_p = S^\circ =$	396.52	398.52	- 2.00	69STU/WES
$C_p^{\circ} =$		129.46			$\Delta_{\epsilon}S^{\circ} =$	0,000	-281.88	2100	0,010,1110
•					$\Delta_{\mathbf{f}}G^{\circ} =$		- 79.92		
Liquid pha	se				$lnK_f =$		32.24		
$\Delta_i H^\circ =$	-251.80	-275.60	23.80	69HU/SIN					
$C_p^{\circ} =$		201.76		-,	Liquid phas	se			
					$\Delta_i H^\circ =$		-225.86		
					$C_p^{\circ} =$	198.24	204.40	-6.16	75RAK/GUT
					$S^{\circ} = \Delta_{f}S^{\circ} =$	237.32	291.82 388.58	54.50	75RAK/GUT
					$\Delta_{\rm f}G^{\circ} =$		- 110.01		
									

TABLE 51. Chlorides (116) - Continued

Tetrachloroe	ethylene Cl) ₂), σ = 4	1		C ₂ Cl ₄	1,1-Dichlor (1×C _d -(C _d -(Cl) ₂), σ =	2	C ₂ H ₂ Cl
(27.08 (0		e – Calculated	= Residual	Reference	(= == (,, ,	re – Calculated		Reference
Gas phase $ \Delta_t H^\circ = \\ C_t^\circ - \\ S^\circ = \\ \Delta_t S^\circ = \\ \Delta_t G^\circ = \\ \ln K_t = $	- 10.80 94.93 340.83	-23.02 93.72 339.29 -118.13 12.20 -4.92	12.22 1.21 1.54	26MAT 69STU/WES 69STU/WES	Gas phase $ \Delta_t H^\circ = C_p^\circ - S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	2.60 67.03 288.07	14.81 68.24 285.17 - 79.86 38.62 - 15.58	- 12.21 1.21 2.90	59HIL/MCD 69STU/WES 69STU/WES
Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t C^\circ - \ln K_t =$	-50.60 146.48	-64.16 152.94 230.70 -226.72 3.44 -1.39	13.56 6.46	53SMI/BJE 82GRO/ING	Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ - \ln K_t =$	se - 24.10 111.29 201.54	-10.33 104.84 201.54 -163.48 38.41 -15.50	- 13.77 6.45 0.00	71MAN/RIN 59HIL/MCD 59HIL/MCD
Chloroethyle (1×C _d -(1		C _d -(H)(Cl)), σ	= 1	C₂H₃Cl	1,2-Dichlor (2×C _d -(Ľ) ×cis corr−(X]	(X) , $\sigma = 2$	C₂H₂CI
	Literatur	e – Calculated	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	35.30 53.72 263.93	30.69 54.13 263.37 - 55.45 47.22 - 19.05	4.61 -0.41 0.56	62LAC/GOT 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t C^\circ =$ $\ln K_t =$	4.60 65.05 289.53	4.74 65.50 289.94 - 75.09 27.13 - 10.94	- 0.14 - 0.45 - 0.41	47KET/VAN 69STU/WES 69STU/WES
2-Chloro-1- (1 × C _d -(0	C)(Cl))+(1	× C-(H) ₃ (C))			Liquid phas $\Delta_t H^\circ = C_p^\circ =$	se - 26.40 113.80	- 25.34 113.24	- 1.06 0.56	53SMI/BJE 34MEH2
Gas phase Δ _t H° =	-21.00	e – Calculated	0.00	Reference 70SHE/ROZ	1,2-Dichloro (2×C _d -(H)(Cl)), σ	= 2		C₂H₂Cl₁
						Literatur	e – Calculated	= Residual	Reference
3-Chlore-1- (1×C _d -(1	$H)_2)+(1\times$	C _d -(H)(C))+(1		C_3H_3CI $CI)), \sigma = 1$ Reference	Gas phase $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ - \Delta_t G^\circ = \ln K_t = K_t^\circ = K_t^\circ$	5.00 66.65 289.90	8.74 65.50 289.94 - 75.09 31.13 - 12.56	-3.74 1.15 -0.04	47KET/VAN 69STU/WES 69STU/WES
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	75.35 306.64	-6.81 77.65 307.81 -147.32 37.11 -14.97	-2.30 -1.17	69STU/WES 69STU/WES	Liquid phas $\Delta_t H^\circ = C_p^\circ =$	se -24.30 112.97	- 25.34 113.24	1.04 - 0.27	53SMI/BJE 34MEH2

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TABLE 51. Chlorides (116) - Continued

TABLE 51. Chlorides (116) - Continued

Trichloroethy (1×C _d -(H)	rlene)(Cl)) + (1 × 0	C _d -(Cl) ₂), σ	= 1	C ₂ HCl ₃	Hexachlorok (6×C _B -(0		ontinued) (6× <i>ortho</i> corr	-(Cl)(Cl)), σ	C_6Cl
	Literature –	· Calculated =	= Residual	Reference	Literature – Calculated = Residual		Reference		
Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	-8.00 80.21 324.80	-7.14 79.61 323.26 -87.96 19.09 -7.70	-0.86 0.60 1.54	44MCD 69STU/WES 69STU/WES	Liquid phas $ \Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = InK_{f} = $	e 111.45	-109.20 211.62 332.82 -370.54 1.28 -0.51	- 2.25	69PLA/GLA
Liquid phase $\Delta_t H^\circ = C_p^\circ =$	- 44.40 124.68	-44.75 133.09	0.35 -8.41	53SMI/BJE 33TRE/WAT	Solid phase $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S$	141.77 201.29 260.24	- 141.00 201.30 260.22 - 443.14 - 8.88	- 0.77 - 0.01 0.02	83PLA/SIM 58HIL/KRA 58HIL/KRA
1, 2,3-Trichlo (1 × C–(H)) ₂ (C)(Cl))+(1×C _d -(C)(C	Cl)) + (1 × C _d = Residual	C ₃ H ₃ Cl ₃ (H)(Cl)) Reference	$lnK_f =$ Chlorobenze	Pne Pne	3.58		C₄H₅C
Gas phase Δ _f H° =		- 70.14				CI)(C _B) ₂) +	· (5×C _B -(H)(C		Reference
Liquid phase $\Delta_t H^\circ = -\frac{1}{1-\text{Chloropro}}$ $(1 \times \text{C-}(\text{H})$	- 101.80 	-101.80 C ₁ -(C))+(1	0.00 × C ₁ -(Cl)), σ	69HU/SIN C ₃ H ₃ Cl = 3	Gas phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	50.90 98.03 313.46	52.02 97.38 312.87 - 159.49 99.57 - 40.17	-1.12 0.65 0.59	68WAD 69STU/WES 69STU/WES
		– Calculated		Reference	Liquid phas				
Gas phase $C_p^{\circ} = S^{\circ} = \Delta_p S^{\circ} = -1$	71.96 284.51	71.96 284.51 40.06	0.00 0.00	69STU/WES 69STU/WES	$\Delta_{t}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = 0$	10.50 150.08 197.48	8.60 148.67 199.82 -272.53 89.86 -36.25	1.90 1.41 -2.34	54HUB/KNO 37STU 37STU
Hexachlorol (6 × C _B -(0	Cl)(C _B) ₂)+(6	5× <i>ortho</i> corr − Calculated	:-(Cl)(Cl)), σ l = Residual	C ₆ Cl ₆ = 12 Reference		Cl)(C _B) ₂) + I) ₃ (C))	zene; p-Chlorot · (4×C _B (H)(C	$(B)_2) + (1 \times C_{B} -$	
Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	-44.70 175.31 441.20	-45.18 175.98 441.82 -261.54 32.80 -13.23	0.48 -0.67 -0.62	83PLA/SIM 69STU/WES 69STU/WES	Gas phase $\Delta_t H^\circ = C_\rho^\circ =$	Literatu	19.59 119.25	= Residual	Reference

 $\ln K_{\rm f} =$

- 13.23

C₈H₉Cl

Reference

TABLE 51. Chlorides (116) - Continued

1-Chloro-4-methylbenzene; p-Chlorotoluene (Continued)	C ₇ H ₇ C
$(1 \times C_B - (Cl)(C_B)_2) + (4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (C)(C_B)_2) + (1 \times C_B)_2 + ($	۲
$(1\times C-(H)_3(C))$	

	Literature – Calculated = Residual						
Liquid pha	ase						
$\Delta_t H^\circ =$	19.90	-28.01	8.11	53SMI/BJE			
$C_p^{\circ} = S^{\circ} =$		172.57					
s° =		234.75					
$\Delta_t S^\circ =$		- 373.91					
$\Delta_{\rm f}G^{\circ} =$		83.47					
$lnK_f =$		-33.67					

1-Chloro-4-ethylbenzene (Continued) C₈H₉Cl $(1 \times C_B - (Cl)(C_B)_2) + (4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (C)(C_B)_2) +$ $(1 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)(C_B))$

	Literatuı	Reference		
Liquid pha	ase			
$\Delta_{\rm f}H^{\circ} =$	-51.76	-52.82	1.06	54HUB/KNO
$C_p^{\circ} =$		195.47		
S° =		282.15		
$\Delta_f S^\circ =$		-462.83		
$\Delta_f G^{\circ} =$		85.17		
$lnK_f =$		-34.36		

 $(5 \times C_B - (H)(C_B)_2) + (1 \times C_B - (C)(C_B)_2) + (1 \times C - (H)_2(C)(C_B)) +$

Literature - Calculated = Residual

C7H7Cl Benzyl chloride $(5 \times C_B - (H)(C_B)_2) + (1 \times C_B - (C)(C_B)_2) + (1 \times C - (H)_2(C_B)(Cl))$

Literature – Calculated = Residual					
10.00	40.00	0.00	TO COVEN		
18.90	18.90	0.00	70COX/PIL		
e					
- 32.60	- 32.60	0.00	56KIR		
		e	B		

(1-Chloroethyl)benzene

 $(1\times C-(H)_2(C)(Cl))$

Gas phase $\Delta_t H^\circ = C_p^\circ =$		1.90 140.94		
Liquid pha		£1 75	C 45	COLLICIA
	- 38.20		-0.45	69HU/SIN
$\Delta_{f}S^{\circ} =$		- 468.46		
$\Delta_f G^\circ =$		87.92		
$lnK_f =$		-35.47		
$\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^$	- 58.20	87.92	- 6.45	69HU/SIN

1-Chloro-2-ethylbenzene CaH₂Ci $(1 \times C_B - (Cl)(C_B)_2) + (1 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)(C_B)) +$ $(1 \times C_B - (C)(C_B)_2) + (4 \times C_B - (H)(C_B)_2) +$ $(1 \times ortho \ corr-(alk)(X))$

	Literature – Calculated = Residual					
Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 6.70	0.76 144.86	- 7.46	49DRE/MAR		
Liquid pha	ise					
$\Delta_{i}H^{\circ} =$	-54.10	- 46.52	−7.58	54HUB/KNO		
$C_p^{\circ} =$		195.47				
S° =		282.15				
$\Delta \epsilon S^{\circ} =$		-462.83				

1-Chloronaphthalene C₁₀H₇Cl $(1 \times C_B - (Cl)(C_B)_2) + (7 \times C_B - (H)(C_B)_2) + (2 \times C_{BF} - (C_{BF})(C_B)_2)$

	Literatur	Reference							
Gas phase									
$\Delta_{f}H^{\circ} =$	119.60	119.84	-0.24	70COX/PIL					
$C_p^{\circ} =$		124.60							
Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	se 54.40	56.58 213.07 246.48 - 379.40 169.70 - 68.46	-2.18	56SMI					

C₈H₉Cl 1-Chloro-4-ethylbenzene $(1 \times C_B - (CI)(C_B)_2) + (4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (C)(C_B)_2) +$ $(1 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)(C_B))$

91.47

-36.90

 $\Delta_{\rm f}G^{\circ} =$

 $lnK_f =$

	Literature	– Calculated	Reference	
Gas phase $\Delta_t H^\circ = C_\rho^\circ =$	-3.64	-1.75 144.86	- 1.89	49DRE/MAR

TABLE 51. Chlorides (116) - Continued

Tr 61	O1 1 . 1 1	(110)	0 4 1
I ABLE 31	. Chlorides	(110) -	Continuea

2-Chloronap (1×C _B -(C		$7 \times C_B - (H)(C_B$	$(2 \times C_{BF})$	$C_{10}H_7CI$ - $(C_{BF})(C_B)_2)$		$H)(C_B)_2) +$	$(2 \times C_B - (Cl)(Cl))$, $\sigma = 2$	_B) ₂) +	C ₆ H ₄ Cl ₂
	Literature	- Calculated =	Residual	Reference	`		re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	137.20	119.84 124.60	17.36	70COX/PIL	Gas phase $\Delta_t H^\circ = C_p^\circ =$	25.50 113.80	16.18 113.10	9.32 0.70	49DRE/MAR 69STU/WES
Liquid phase $\Delta_l H^\circ = C_p^\circ = S^\circ =$	e	56.58 213.07 246.48			$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$	343.46	341.64 176.92 68.93 27.81	1.82	69STU/WES
$\Delta_{f}S^{\circ} = \\ \Delta_{f}G^{\circ} = \\ \ln K_{f} = $		- 379.40 169.70 - 68.46			Liquid phas $ \Delta_t H^\circ = C_p^\circ = S^\circ = $	e – 20.90	- 21.76 161.26 226.42	0.86	54HUB/KNO
Solid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ =$	55.20	41.91 179.06 190.62 – 435.26	13.29	56SMI	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-292.13 65.34 -26.36		
$\Delta_{\rm f}G^{\circ} = \\ \ln K_{\rm f} = \\ -$		171.68 - 69.26			1,4-Dichloro		(2×C _B -(Cl)(C	$_{\rm B})_2),\sigma=2$	C ₄ H ₄ Cl ₂
1,2-Dichlore	obenzene			Ċ₅H₄Cl₂		Literatu	re – Calculated	= Residual	Reference
	corr-(Cl)($(2 \times C_B - (Cl)(C_l))$, $\sigma = 2$ e - Calculated		Reference	Gas phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	22.18 113.89 336.69	21.18 113.10 341.64	1.00 0.79 - 4.95	61WAL/SMI 69STU/WES 69STU/WES
Gas phase $\Delta_t H^\circ = C_p^\circ =$	29.63 113.47	30.68 113.10	-1.05 0.37	49DRE/MAR 69STU/WES	$\Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = \frac{1}{2}$	330.09	- 176.92 - 73.93 - 29.82	-4.93	09310/WE3
$S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t =$	341.46	341.64 -176.92 83.43 -33.65	-0.18	69STU/WES	Liquid phas $ \Delta_t H^\circ = C_\rho^\circ = S^\circ = $	ee	- 31.76 161.26 226.42		
Liquid phase $\Delta_t H^\circ - C_p^\circ =$	se - 18.07	- 17.76 161.26	-0.31	54HUB/KNO	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-292.13 55.34 -22.32		Page 14 (1976)
$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = -\infty$		226.42 - 292.13 69.34 - 27.97			Solid phase $ \Delta_{\ell}H^{\circ} = \\ C_{p}^{\circ} = \\ S^{\circ} = \\ \Delta_{\ell}S^{\circ} = \\ \Delta_{f}G^{\circ} = $	-42.84 147.76 175.41	- 37.88 147.62 177.74 - 340.81 63.73	4.96 0.14 2.33	54HUB/KNO 76DWO/FIG 76DWO/FIG

 $lnK_f =$

C₁₂H₈Cl₂

C₆HCl₅

TABLE 51. Chlorides (116) - Continued

4,4'-Dichlorobiphenyl (Continued)

2,5-Dichlorostyrene	C ₈ H ₆ Cl ₂
$(1 \times C_{d} - (H)_{2}) + (1 \times C_{d} - (H)(C_{B})) + (1 \times C_{B} - (C_{d})(C_{B})_{2}) +$	
$(3 \times C_{B}-(H)(C_{B})_{2}) + (2 \times C_{B}-(Cl)(C_{B})_{2}) +$	
$(2 \times ortho \ corr-(alk)(X))$	

	Literatur	Literature - Calculated = Residual							
Gas phase									
$\Delta_t H^\circ =$		91.16							
$C_{\rho}^{\circ} =$		153.53		ut					
Liquid phas $\Delta_t H^\circ =$	se 35.90	35.73	0.17	58SIN/STU					
$C_p^{\circ} =$		208.06							
S° =		288.00							
$\Delta_f S^\circ =$		-372.60							
$\Delta_{\rm f}G^{\circ} =$		146.82							
$lnK_f =$		- 59.23							

$\begin{array}{c} \textbf{2.2'-Dichlorobiphenyl} & \textbf{C}_{12}\textbf{H}_{8}\textbf{Cl}_{2} \\ (8 \times \textbf{C}_{B} - (\textbf{H})(\textbf{C}_{B})_{2}) + (2 \times \textbf{C}_{B} - (\textbf{Cl})(\textbf{C}_{B})_{2}) + (2 \times \textbf{C}_{B} - (\textbf{C}_{B})_{3}) + \\ (1 \times \textit{ortho} \ \textit{corr} - (\textbf{Cl})(\textbf{Cl'})) \end{array}$

	Literature	Literature - Calculated = Residual Refere			
Gas phase					
$\Delta_{\rm f} H^{\circ} =$	127.90	127.74	0.16	64SMI/GOR	
C _p ° =		193.78			
Liquid phas	se				
$\Delta_{i}H^{\circ} =$		43.30			
C _p ° =		286.12			
Solid phase					
$\Delta_{\rm f}H^{\circ} =$	31.70	30.30	1.40	64SMI/GOR	
$C_n^{\circ} =$		224.70			
S° =		256.74			
Δ _r S° -		557.40			
$\Delta_f G^\circ =$		196.49			
$lnK_f =$		- 79.26			

$\begin{array}{ll} \textbf{4,4'-Dichlorobiphenyl} & C_{12}H_8Cl_2 \\ (8\times C_B-(H)(C_B)_2) + (2\times C_B-(Cl)(C_B)_2) + (2\times C_B-(C_B)_3) \end{array}$

	Literature	Literature - Calculated = Residual			
Gas phase					
$\Delta_t H^\circ =$	121.10	119.74	1.36	64SMI/GOR	
$C_p^{\circ} =$		193.78			
Liquid phas $\Delta_t H^\circ = C_p^\circ =$	se	35.30 286.12			

$(8 \times C_{B}-(F$			$_{\rm B})_2)+(2\times C_{\rm B}-$	$(C_B)_3)$
	Literature	- Calculated	= Residual	Reference
Solid phase	17.20	22.20	£ 00	(40) #JGOD
$\Delta_{\rm f}H^{\rm o} =$	17.30	22.30	-5.00	64SMI/GOR
C_p° –		224.70		
S° =		256.74		
$\Delta_f S^\circ =$		-557.40		
$\Delta_{\mathbf{f}}G^{\circ} =$		188.49		

$\begin{array}{ll} \textbf{1.2.4.5-Tetrachloro-3.6-dimethylbenzene} & \textbf{C_8H_6Cl_4} \\ (2 \times C - (H)_3(C)) + (2 \times C_B - (C)(C_B)_2) + (4 \times C_B - (Cl)(C_B)_2) + \\ (2 \times \textit{ortho} \ \textit{corr} - (Cl)(Cl)) + (4 \times \textit{ortho} \ \textit{corr} - (alk)(X)) \end{array}$

-76.03

Literat	ture – Calculated =	Residual	Reference
Gas phase			
$\Delta_l H^{\hat{\alpha}} =$	-76.32		
$C_p^{\circ} =$	188.28		
Liquid phase			
$\Delta_{\rm f}H^{\circ} =$	- 132.50		
$C_p^{\circ} =$	234.24		
S° =	349.48		
$\Delta_f S^{\circ} =$	-534.10		
$\Delta_{\rm f}G^{\circ} =$	26.74		
$lnK_f =$	- 10.79		
Solid phase			
$\Delta_{\rm f}H^{\circ} = -173.90$	-176.68	2.78	69HU/SIN
$C_{\rho}^{\circ} =$	222.58		
S° -	275.86		
$\Delta_f S^o =$	-607.72		
$\Delta_{f}G^{\circ} =$	4.51		
$lnK_f =$	- 1.82		

Pentachlorobenzene $(1\times C_B-(H)(C_B)_2)+(5\times C_B-(Cl)(C_B)_2)+\\ (4\times ortho\ corr-(Cl)(Cl))+(1\times meta\ corr-(Cl)(Cl))$

	Literatui	e – Calculated	= Residual	Reference
Gas phase				
$\Delta_i H^{\circ} =$	-40.00	-38.34	-1.66	85PLA/SIM
C_p^{α} -		160.26		
	· · · · · · · · · · · · · · · · · · ·			
Liquid phas	se			
$\Delta_t H^{} =$		 8б.84		
$C_{p}^{\circ} =$		199.03		
S° =		306.22		
$\Delta_t S^\circ =$		-350.94		
$\Delta_{r}G^{\circ} =$		17.79		
$lnK_f =$		-7.18		

TABLE 51. Chlorides (116) - Continued

	$I)(C_B)_2)+($	ontinued) 5 × C _B –(Cl)(C _B Cl)) + (1 × meta		C₄HCl₅	4-Chloroph $(4 \times C_B - (1 \times O - (1 \times O + (1 \times $	$(H)(C_B)_2) +$	(1×C _B -(Cl)(C	$_{\rm B})_2)+(1\times {\rm C_{B^{-1}}}$	C_6H_5ClO (O)(C_B) ₂) +
	Literature	e – Calculated =	= Residual	Reference	_	Literatu	re – Calculated	= Residual	Reference
Solid phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = C_p^\circ = C_p^\circ = C_p^\circ $	- 120.40	-115.47 187.88 239.60 -417.56	-4.93	85PLA/SIM	Gas phase $\Delta_f H^\circ = C_\rho^\circ =$	- 145.80	- 126.84 117.79	-18.96	38WOL/WEG
$\Delta_f G^\circ = \ln K_f =$		9.02 - 3.64			$C_p^{\circ} =$	se -181.30	- 196.92 210.34	15.62	53SMI/BJE
		×C-(H)(C) ₂ (0 b) rsc)	CI))+	C ₆ H ₁₁ Cl	$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f =$		204.25 - 370.62 - 86.42 34.86		
	Literatur	e – Calculated	= Residual	Reference	Solid phase $\Delta_t H^\circ =$		- 204.13	6.42	52CMI/DIE
Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 163.70	- 159.15 126.63	-4.55	70COX/PIL	$\Delta_{f}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$	- 197.70	-204.13 143.03 164.58 -410.30 -81.80 33.00	6.43	53SMI/BJE
Liquid phas $\Delta_t H^\circ = C_p^\circ =$	se 207.20	- 201.88 191.91	-5.32	56KIR		,3-propaned H)(C))+(2	iiol × C-(H)2(O)(C	'))+(1×C-(H	C ₃ H ₇ ClO ₂)(C) ₂ (Cl))
3-Chlorophe	enol			C₅H₅ClO		Literatur	re – Calculated	= Residual	Reference
$(4 \times C_B - (1 \times O -$	$H)(C_B))$	(1 × C _B -(Cl)(C		(O)(C _B) ₂)+ Reference	Gas phase $\Delta_t H^\circ = C_p^\circ =$		- 440.07 111.98		
Gas phase $\Delta_t H^\circ = C_p^\circ =$	-153.30	126.84 117.79	- 26.46	38WOL/WEG	Liquid pha $\Delta_t H^\circ = C_p^\circ =$	se - 517.50	- 525.77 222.58	8.27	54BJE/SMI
Liquid phas $\Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} =$	se 189.30	- 196.92 210.34 204.25 - 370.62	7.62	53SMI/BJE	(1×C-(1	H) ₂ (O)(C)) ·	+ (1 × C–(H)(C + (2 × O–(H)(C))	
$\Delta_f G^\circ = \ln K_f =$		-86.42 34.86			******	Literatui	re Calculated	= Residual	Reference
Solid phase $\Delta_t H^\circ = C_p^\circ =$	- 206.40	-204.13 143.03	-2.27	53SMI/BJE	Gas phase $\Delta_t H^\circ = C_p^\circ =$		-447.11 114.14		
$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$		164.58 -410.30 -81.80 33.00			Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$	se - 525.30	-533.30 236.51 194.81 -595.94	8.00	54BJE/SMI
					$\Delta_{\rm f}G^{\circ} = \ln K_{\rm f} =$		-355.62 143.46		

TABLE 51. Chlorides (116) - Continued

$(2 \times C - (H)_2)(1 \times O - (H))(0$								
I	Literature -	- Calculated =	= Residual	Reference	Liter	ature – Calculated	= Residual	Reference
						· ····		
Sas phase				#4.00YI PYY	Gas phase			
•	318.40	- 324.33	5.93	70COX/PIL	$\Delta_t H^{\circ} =$	-336.54		
$C_p^{\circ} =$		113.18			$C_p^{\circ} =$	153.92	<u> </u>	
iquid phase					Liquid phase			
	385.30	-392.90	7.60	54BJE/SMI	$\Delta_i H^\circ =$	-442.80		
$C_{p}^{\circ} =$		221.99			$C_n^{\circ} =$	284.60		
S° =		222.60			S° =	235.28		
$\Delta_f S^\circ =$		-511.83			Δ ₆ S° =	-488.32		
$\Delta_f G^\circ =$		-240.30			$\Delta_f G^\circ =$	-297.21		
$\ln K_{\rm f} =$		96.93			$\ln K_{\rm f} =$	119.89		
2 DI II 1				CHOLO	Call at an			
,3-Dichloro-1-		(1 2 0 (11)/0)	((1)) (4::	C ₃ H ₆ Cl ₂ O	Solid phase	0 447.44	00.14	5201 ST 10-10-
		$(1 \times C - (H)(C)$	₁₂ (C1))+(1×	C-(H) ₂ (O)(C))+	$\Delta_t H^\circ = -427.3$		20.14	53SMI/BJE
$(1 \times O - (H))$	(C))				$C_p^{\circ} =$	165.28		
	~ 1.			5 . c	S° -	192.66		
ı	Literature -	Calculated =	= Residual	Reference	$\Delta_{r}S^{\circ} =$	- 530.94		
					$\Delta_{\rm f}G^{\circ} =$	- 289.14		
					$lnK_f =$	116.64		
Gas phase								
$\Delta_i H^\circ = -3$	316.30	-317.29	0.99	70COX/PIL				
$C_p^{\circ} =$		111.02						
*								
					2.6-Dichloro-1.4-be	nzenediol		CHCL
					2,6-Dichloro-1,4-be		u)2) + (2 × Co-	C ₆ H ₄ Cl ₂
iquid phase			,		$(2\times C_B-(H)(C_B)$	$(2 \times C_{B} - (Cl)) (C_l)$		$C_6H_4Cl_2$ $C_6(O)(C_B)_2) +$
	381 50	395 37	3 27	SARIE/SMI	$(2\times C_B-(H)(C_B)$			$C_6H_4Cl_2$ $C_8(O)(C_B)_2) +$
$\Delta_i H^\circ = -3$	381.50	-385.37 208.06	3.87	54BJE/SMI	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$) + (2×C _B -(Cl)(C _l + (1× <i>meta</i> corr-(C	CI)(CI))	-(O)(C _B) ₂)+
	381.50	-385.37 208.06	3.87	54BJE/SMI	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$	$(2 \times C_{B} - (Cl)) (C_l)$	CI)(CI))	C ₆ H ₄ Cl ₂ (O)(C _B) ₂) + Reference
$\Delta_t H^\circ = -3$ $C_p^\circ = -3$		208.06	3.87	54BJE/SMI C₀H₄Cl₂O₂	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$) + (2×C _B -(Cl)(C _l + (1× <i>meta</i> corr-(C	CI)(CI))	
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} = -3$ 2,3-Dichloro-1,	,4-benzene	208.06 diol		C ₆ H ₄ Cl ₂ O ₂	(2×C _B -(H)(C _B) (2×O-(H)(C _B)) Liter) + (2×C _B -(Cl)(C _l + (1× <i>meta</i> corr-(Cature – Calculated	CI)(CI))	(O)(C _B) ₂)+ Reference
$\Delta_t H^\circ = -3$ $C_p^\circ = -3$ 2,3-Dichloro-1, $(2 \times C_B - (H))$,4-benzene (C _B) ₂) + (2	208.06 $diol \times C_B-(Cl)(C_B$	a) ₂)+(2×C _B -	C ₆ H ₄ Cl ₂ O ₂	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$	$\begin{array}{l} (2 \times C_B - (CI)(C_I) + (1 \times meta \text{ corr} - (CI)(C_I) + (1 $	CI)(CI)) = Residual	-(O)(C _B) ₂)+
$\Delta_{i}H^{\circ} = -3$ $C_{\rho}^{\circ} = -3$ $C_{\rho}^{\circ} = -3$ 2,3-Dichloro-1, $(2 \times C_{B} - (H))(3 \times C_{B} - (H))(4 \times$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	(2×C _B -(H)(C _B)) (2×O-(H)(C _B)) Liter Gas phase) + (2×C _B -(Cl)(C _l + (1× <i>meta</i> corr-(Cature – Calculated	CI)(CI)) = Residual	(O)(C _B) ₂)+ Reference
$\Delta_i H^\circ = -3$ $C_p^\circ =$ 2,3-Dichloro-1, $(2 \times C_B - (H))(0)$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 $diol \times C_B-(Cl)(C_B$	s) ₂) + (2 × C _B - Cl)(Cl))	C ₆ H ₄ Cl ₂ O ₂	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter $Gas phase$ $\Delta_t H^\circ = -331.5$ $C_p^\circ =$	$\begin{array}{l} (2 \times C_B - (CI)(C_I) + (1 \times meta \text{ corr} - (CI)(C_I) + (1 $	CI)(CI)) = Residual	(O)(C _B) ₂) + Reference
$\Delta_i H^\circ = -3$ $C_p^\circ =$ 2,3-Dichloro-1, $(2 \times C_B - (H))(0)$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_l H^\circ = -331.5$ $C_p^\circ =$ Liquid phase) + (2×C _B -(Cl)(C _I +(1×meta corr-(Cature - Calculated at the corr-(Cature - Calculated at the corr-(Cature - Cature -	CI)(CI)) = Residual	(O)(C _B) ₂) + Reference
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} = -3$ 2,3-Dichloro-1, $(2 \times C_{B}-(H))$ $(2 \times O-(H))$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ =$) + (2×C _B -(Cl)(C _I +(1×meta corr-(Cature - Calculated and 153.92	CI)(CI)) = Residual	(O)(C _B) ₂) + Reference
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} = -3$ 2,3-Dichloro-1, $(2 \times C_{B}-(H))(2 \times O-(H))(3 \times O-(H))$ Gas phase	,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	diol × C _B -(Cl)(C _B ortho corr-(C	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$)-1 (2×C _B -(Cl)(C _I +(1×meta corr-(Cl)) ature - Calculated 1 - 341.54 153.92 - 432.80 284.60	CI)(CI)) = Residual	(O)(C _B) ₂) + Reference
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} =$ 2,3-Dichloro-1, $(2 \times C_{B}-(H))$ $(2 \times O-(H))$ Gas phase $\Delta_{i}H^{\circ} =$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$) + (2×C _B -(Cl)(C _I +(1×meta corr-(Cl)) ature - Calculated 1 - 341.54 153.92 - 432.80 284.60 235.28	CI)(CI)) = Residual	(O)(C _B) ₂) + Reference
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} = -3$ 2,3-Dichloro-1, $(2 \times C_{B}-(H))$ $(2 \times O-(H))$ Gas phase	,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	diol × C _B -(Cl)(C _B ortho corr-(C	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_{B^{-}}(H)(C_{B}))$ $(2 \times O^{-}(H)(C_{B}))$ Liter Gas phase $\Delta_{t}H^{\circ} = -331.5$ $C_{p}^{\circ} =$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $S^{\circ} = \Delta_{t}S^{\circ} =$	-432.80 284.60 235.28 -488.32	CI)(CI)) = Residual	(O)(C _B) ₂) + Reference
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} =$ 2,3-Dichloro-1, $(2 \times C_{B}-(H))$ $(2 \times O-(H))$ Gas phase $\Delta_{i}H^{\circ} =$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	- 432.80 - 235.28 - 488.32 - 24 (CI)(C _I +(1×meta corr-(C)) - 341.54 153.92	CI)(CI)) = Residual	(O)(C _B) ₂) + Reference
$\Delta_{i}H^{\circ} = -3$ $C_{\rho}^{\circ} =$ 2,3-Dichloro-1, $(2 \times C_{B} - (H))(2 \times O - (H))(3 \times O - (H))(4 \times O - (H))(4 \times O - (H))(5 \times O - (H))(6 \times O - (H))(7 \times O - (H))(7$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_{B^{-}}(H)(C_{B}))$ $(2 \times O^{-}(H)(C_{B}))$ Liter Gas phase $\Delta_{t}H^{\circ} = -331.5$ $C_{p}^{\circ} =$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $S^{\circ} = \Delta_{t}S^{\circ} =$	-432.80 284.60 235.28 -488.32	CI)(CI)) = Residual	(O)(C _B) ₂) + Reference
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} = -3$ $C_{p}^{\circ} = -3$ 2,3-Dichloro-1, $(2 \times C_{B} - (H))$ $(2 \times O - (H))$ Gas phase $\Delta_{i}H^{\circ} = C_{p}^{\circ} = -3$ Liquid phase	,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	- 432.80 - 235.28 - 488.32 - 24 (CI)(C _I +(1×meta corr-(C)) - 341.54 153.92	CI)(CI)) = Residual	(O)(C _B) ₂) + Reference
$\Delta_i H^\circ = -3$ $C_p^\circ =$ 2,3-Dichloro-1, $(2 \times C_B - (H))$ $(2 \times O - (H))$ Gas phase $\Delta_i H^\circ = C_p^\circ =$ Liquid phase	,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	- 432.80 - 235.28 - 488.32 - 24 (CI)(C _I +(1×meta corr-(C)) - 341.54 153.92	CI)(CI)) = Residual	(O)(C _B) ₂) + Reference
$\Delta_i H^\circ = -3$ $C_\rho^\circ =$ 2,3-Dichloro-1, $(2 \times C_B - (H))$ $(2 \times O - (H))$ Gas phase $\Delta_i H^\circ = C_\rho^\circ =$ Liquid phase	,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$	- 432.80 - 235.28 - 488.32 - 24 (CI)(C _I +(1×meta corr-(C)) - 341.54 153.92	CI)(CI)) = Residual	(O)(C _B) ₂) + Reference
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} =$ 2,3-Dichloro-1, $(2 \times C_{B}-(H))$ $(2 \times O-(H))$ Gas phase $\Delta_{i}H^{\circ} =$ $C_{p}^{\circ} =$ Liquid phase $\Delta_{i}H^{\circ} =$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ Solid phase	-432.80 235.28 -488.32 -287.21 115.86	Cl)(Cl)) = Residual 10.04	(O)(C _B) ₂) + Reference 27COO/COO
$C_p^{\circ} =$ 2,3-Dichloro-1, $(2 \times C_B - (H))(2 \times O - (H))(3 \times O - (H))(4 \times O - (H))(5 \times O - (H))(6 \times O - (H)$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60 235.28	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ Solid phase $\Delta_t H^\circ = -423.5$	- 432.80 - 235.28 - 48.32 - 287.21 - 243.44	CI)(CI)) = Residual	(O)(C _B) ₂)+ Reference
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} =$ 2,3-Dichloro-1, $(2 \times C_{B}-(H))(2 \times O_{P}-(H))(3 \times O_{P}-(H))(4 \times O_{P}-(H))(5 \times O_{P}-(H))(6 \times O_{P}-(H))$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60 235.28 - 488.32	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = \ln K_t =$ Solid phase $\Delta_t H^\circ = -423.5$ $C_p^\circ = $	- 432.80 - 287.21 - 287.21 - 432.80 - 284.60 - 235.28 - 488.32 - 287.21 - 115.86	Cl)(Cl)) = Residual 10.04	(O)(C _B) ₂) + Reference 27COO/COO
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} =$ 2.3-Dichloro-1, $(2 \times C_{B} - (H))(2 \times O - (H))(3 \times O - (H))(4 \times O - (H))(5 \times O - (H))(6 \times O - (H))(6$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60 235.28 - 488.32 - 283.21	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = 1nK_t =$ Solid phase $\Delta_t H^\circ = -423.5$ $C_p^\circ = S^\circ $	- 432.80 - 284.60 - 235.28 - 488.32 - 287.21 - 243.44 - 165.28 - 192.66	Cl)(Cl)) = Residual 10.04	(O)(C _B) ₂) + Reference 27COO/COO
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} =$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60 235.28 - 488.32	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_\rho^\circ =$ Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = A_t S^\circ$	- 432.80 - 284.60 - 235.28 - 488.32 - 287.21 115.86	Cl)(Cl)) = Residual 10.04	(O)(C _B) ₂) + Reference 27COO/COO
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} =$ 1.3-Dichloro-1, $(2 \times C_{B} - (H))(2 \times O - (H))(3 \times O - (H))(4 \times O - (H))(5 \times O - (H))(6 \times O - (H))(6$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60 235.28 - 488.32 - 283.21	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ$	2)+1 (2×C _B -(Cl)(C _I +(1×meta corr-(Cl))+(1×meta corr-(Cl)) ature - Calculated (1) 3) -341.54 153.92 -432.80 284.60 235.28 -488.32 -287.21 115.86 3) -443.44 165.28 192.66 -530.94 -285.14	Cl)(Cl)) = Residual 10.04	(O)(C _B) ₂) + Reference 27COO/COO
$\Delta_{l}H^{\circ} = -3$ $C_{p}^{\circ} =$ 2.3-Dichloro-1, $(2 \times C_{B} - (H))(2 \times O - (H))(3 \times O - (H))(4 \times O - (H))(5 \times O - (H))(6 \times O - (H))(6$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60 235.28 - 488.32 - 283.21	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_\rho^\circ =$ Liquid phase $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = A_t S^\circ$	- 432.80 - 235.28 - 488.32 - 287.21 - 215.86 - 235.28 - 488.32 - 287.21 - 432.46 - 235.28 - 488.32 - 287.21 - 432.46 - 235.28 - 488.32 - 287.21 - 287.	Cl)(Cl)) = Residual 10.04	(O)(C _B) ₂) + Reference 27COO/COO
$C_p^{\alpha} = -3$ $C_p^$,4-benzene (C _B)2) + (2 C _B)) + (1 × Literature	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60 235.28 - 488.32 - 283.21 114.24	a) ₂) + (2 × C _B - I)(CI)) = Residual	C ₆ H ₄ Cl ₂ O ₂ -(O)(C _B) ₂) + Reference	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ$	2)+1 (2×C _B -(Cl)(C _I +(1×meta corr-(Cl))+(1×meta corr-(Cl)) ature - Calculated (1) 3) -341.54 153.92 -432.80 284.60 235.28 -488.32 -287.21 115.86 3) -443.44 165.28 192.66 -530.94 -285.14	Cl)(Cl)) = Residual 10.04	(O)(C _B) ₂) + Reference 27COO/COO
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} =$ 2,3-Dichloro-1, $(2 \times C_{B} - (H))(2 \times C_{B} - (H))(3 \times C_{B} + (H))(4 \times C$,4-benzene (C _B) ₂) + (2 (C _B)) + (1 ×	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60 235.28 - 488.32 - 283.21 114.24 - 438.94	s) ₂) + (2 × C _B - Cl)(Cl))	$C_6H_4Cl_2O_2$ -(O)(C_B) ₂)+	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ$	2)+1 (2×C _B -(Cl)(C _I +(1×meta corr-(Cl))+(1×meta corr-(Cl)) ature - Calculated (1) 3) -341.54 153.92 -432.80 284.60 235.28 -488.32 -287.21 115.86 3) -443.44 165.28 192.66 -530.94 -285.14	Cl)(Cl)) = Residual 10.04	(O)(C _B) ₂) + Reference 27COO/COO
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} =$ 2,3-Dichloro-1, $(2 \times C_{B} - (H))(2 \times C_{B} - (H))(3 \times C_{p}^{\circ})$ Gas phase $\Delta_{i}H^{\circ} = C_{p}^{\circ} =$ $\Delta_{i}G^{\circ} = C_{p}^{\circ} = C_{p}^{\circ} =$ Solid phase $\Delta_{i}H^{\circ} = C_{p}^{\circ} = C_{$,4-benzene (C _B)2) + (2 C _B)) + (1 × Literature	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60 235.28 - 488.32 - 283.21 114.24 - 438.94 165.28	a) ₂) + (2 × C _B - I)(CI)) = Residual	C ₆ H ₄ Cl ₂ O ₂ -(O)(C _B) ₂) + Reference	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ$	2)+1 (2×C _B -(Cl)(C _I +(1×meta corr-(Cl))+(1×meta corr-(Cl)) ature - Calculated (1) 3) -341.54 153.92 -432.80 284.60 235.28 -488.32 -287.21 115.86 3) -443.44 165.28 192.66 -530.94 -285.14	Cl)(Cl)) = Residual 10.04	(O)(C _B) ₂) + Reference 27COO/COO
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} =$ 2,3-Dichloro-1, $(2 \times C_{B}-(H))(2 \times O_{P}-(H))(3 \times O_{P}-(H))(4 \times O_{P}-(H))(5 \times O_{P}-(H))(5 \times O_{P}-(H))(6 \times O_{P}-(H))$,4-benzene (C _B)2) + (2 C _B)) + (1 × Literature	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60 235.28 - 488.32 - 283.21 114.24 - 438.94	a) ₂) + (2 × C _B - I)(CI)) = Residual	C ₆ H ₄ Cl ₂ O ₂ -(O)(C _B) ₂) + Reference	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ$	2)+1 (2×C _B -(Cl)(C _I +(1×meta corr-(Cl))+(1×meta corr-(Cl)) ature - Calculated (1) 3) -341.54 153.92 -432.80 284.60 235.28 -488.32 -287.21 115.86 3) -443.44 165.28 192.66 -530.94 -285.14	Cl)(Cl)) = Residual 10.04	(O)(C _B) ₂) + Reference 27COO/COO
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} =$ 2,3-Dichloro-1, $(2 \times C_{B}-(H))(2 \times C_{B}-(H))(3 \times C_{B})$ Gas phase $\Delta_{i}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{i}H^{\circ} = C_{p}^{\circ} = C_{p}^{\circ} = C_{B}^{\circ} = C_$,4-benzene (C _B)2) + (2 C _B)) + (1 × Literature	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60 235.28 - 488.32 - 283.21 114.24 - 438.94 165.28	a) ₂) + (2 × C _B - I)(CI)) = Residual	C ₆ H ₄ Cl ₂ O ₂ -(O)(C _B) ₂) + Reference	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ$	2)+1 (2×C _B -(Cl)(C _I +(1×meta corr-(Cl))+(1×meta corr-(Cl)) ature - Calculated (1) 3) -341.54 153.92 -432.80 284.60 235.28 -488.32 -287.21 115.86 3) -443.44 165.28 192.66 -530.94 -285.14	Cl)(Cl)) = Residual 10.04	(O)(C _B) ₂) + Reference 27COO/COO
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} =$ 2,3-Dichloro-1, $(2 \times C_{B}-(H))(2 \times O_{-}(H))(3 \times O_{-}(H))(4 \times O_{-}(H))(5 \times O_{-}(H))(6 \times O$,4-benzene (C _B)2) + (2 C _B)) + (1 × Literature	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60 235.28 - 488.32 - 283.21 114.24 - 438.94 165.28 192.66 - 530.94	a) ₂) + (2 × C _B - I)(CI)) = Residual	C ₆ H ₄ Cl ₂ O ₂ -(O)(C _B) ₂) + Reference	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ$	2)+1 (2×C _B -(Cl)(C _I +(1×meta corr-(Cl))+(1×meta corr-(Cl)) ature - Calculated (1) 3) -341.54 153.92 -432.80 284.60 235.28 -488.32 -287.21 115.86 3) -443.44 165.28 192.66 -530.94 -285.14	Cl)(Cl)) = Residual 10.04	(O)(C _B) ₂) + Reference 27COO/COO
$\Delta_{i}H^{\circ} = -3$ $C_{p}^{\circ} =$ 2,3-Dichloro-1, $(2 \times C_{B}-(H))(2 \times O_{-}(H))(3 \times O_{-}(H))(4 \times O_{-}(H))(5 \times O_{-}(H))(6 \times O$,4-benzene (C _B)2) + (2 C _B)) + (1 × Literature	208.06 diol × C _B -(Cl)(C _B ortho corr-(C - Calculated = - 327.04 153.92 - 428.80 284.60 235.28 - 488.32 - 283.21 114.24 - 438.94 165.28 192.66	a) ₂) + (2 × C _B - I)(CI)) = Residual	C ₆ H ₄ Cl ₂ O ₂ -(O)(C _B) ₂) + Reference	$(2 \times C_B - (H)(C_B))$ $(2 \times O - (H)(C_B))$ Liter Gas phase $\Delta_t H^\circ = -331.5$ $C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ$	2)+1 (2×C _B -(Cl)(C _I +(1×meta corr-(Cl))+(1×meta corr-(Cl)) ature - Calculated (1) 3) -341.54 153.92 -432.80 284.60 235.28 -488.32 -287.21 115.86 3) -443.44 165.28 192.66 -530.94 -285.14	Cl)(Cl)) = Residual 10.04	(O)(C _B) ₂) + Reference 27COO/COO

TABLE 51. Chlorides (116) - Continued

2,3,5-Trichloro-1,4-benzenediol	C ₆ H ₃ Cl ₃ O ₂
$(1 \times C_B - (H)(C_B)_2) + (3 \times C_B - (Cl)(C_B)_2) + (2 \times O - (H)(C_B)_2)$)+
$(2 \times C_{B}-(O)(C_{B})_{2}) + (1 \times ortho \text{ corr}-(Cl)(Cl)) +$	
$(1 \times meta \text{ corr-}(Cl)(Cl))$	

Literatu	re – Calculated =	= Residual	Reference
Gas phase			
$\Delta_t H^{\circ} = -339.40$	-362.88	23.48	27COO/COO
$C_p^{\circ} =$	169.64		
Liquid phase			
$\Delta_t H^\circ =$	-459.16		
$C_p^{\circ} =$	297.19		
<i>S</i> ° =	261.88		
$\Delta_{\mathbf{f}}S^{\circ} =$	-507.92		
$\Delta_{\rm f}G^{\circ} =$	-307.72		
$lnK_f =$	124.13		
Solid phase			
$\Delta_{\rm f}H^{\circ} = -440.70$	-473.47	32.77	53SMI/BJE
$C_p^{\circ} =$	178.70		
S° =	213.28		
$\Delta_f S^\circ =$	-556.52		
$\Delta_{\rm f}G^{\circ} =$	-307.54		
$lnK_f =$	124.06		

 $\label{eq:pentachlorophenol} \begin{array}{c} \textbf{C_6HCl_5O} \\ (1 \times O - (H)(C_B)) + (1 \times C_{B} - (O)(C_B)_2) + (5 \times C_{B} - (Cl)(C_B)_2) + \\ (4 \times \textit{ortho} \ \textit{corr} - (Cl)(Cl)) \end{array}$

Literatur	re – Calculated	= Residual	Reference
Gas phase			
$\Delta_{\rm f}H^{\circ} = -225.10$	-212.20	-12.90	70COX/PIL
$C_p^{\circ} =$	180.67		
Liquid phase			
$\Delta_t H^\circ =$	-302.36		
$C_p^{\circ} =$	260.70		
S° =	310.65		
$\Delta_{f}S^{\circ} =$	-449.03		
$\Delta_{\mathbf{f}}G^{\circ} =$	-168.48		
$lnK_f =$	67.96		
Solid phase			
$\Delta_{\rm f} H^{\circ} = -292.50$	-324.25	31.75	58SIN/STU
$C_p^{\circ} =$	196.71		
S° =	247.06		
$\Delta_{\mathbf{f}}S^{\circ} =$	-512.62		
$\Delta_{\mathbf{f}}G^{\circ} =$	-171.41		
$lnK_f =$	69.15		

 $\begin{array}{ll} \textbf{2,3,5,6-Tetrachloro-1,4-benzenediol} & C_{\textbf{6}}H_{2}Cl_{\textbf{4}}O_{\textbf{2}} \\ (4 \times C_{\textbf{B}}-(Cl)(C_{\textbf{B}})_{2}) + (2 \times O-(H)(C_{\textbf{B}})) + (2 \times C_{\textbf{B}}-(O)(C_{\textbf{B}})_{2}) + \\ (2 \times \textit{ontho} \ \textit{corr}-(Cl)(Cl)) + (2 \times \textit{meta} \ \textit{corr}-(Cl)(Cl)) \end{array}$

·	Literatur	e — Calculated =	Residual	Reference
Gas phase				
$\Delta_t H^{\circ} =$		-389.22		
$C_p^{\circ} =$		185.36		
Liquid phas	ie			
$\Delta_{i}H^{\circ} =$		-475.52		
$C_{p}^{\circ} =$		309.78		
s° =		288.48		
$\Delta_f S^\circ =$		- 527.52		
$\Delta_t G^\circ =$		-318.24		
$lnK_f =$		128.38		
Solid phase	ı			
$\Delta_{\mathbf{f}}H^{\circ} =$	-453.60	499.50	45.90	53SMI/BJE
$C_p^{\circ} =$		192.12		
S° =		233.90		
$\Delta_{\rm f} S^{\circ} =$		-582.10		
$\Delta_{\mathbf{f}}G^{\circ} =$		-325.95		
$lnK_f =$		131.48		

 $\begin{array}{l} \textbf{2-Chloro-1,4-benzenediol} & \textbf{C_6H_5ClO_2} \\ (3 \times C_B-(H)(C_B)_2) + (1 \times C_B-(Cl)(C_B)_2) + (2 \times O-(H)(C_B)) + \\ (2 \times C_B-(O)(C_B)_2) \end{array}$

Literatu	re – Calculated	= Residual	Reference
Gas phase			
$\Delta_{\rm f} H^{\circ} = -314.00$	-305.70	-8.30	27COO/COO
$C_{\rho}^{\circ} =$	138.20		
Liquid phase			
$\Delta_t H^\circ =$	-402.44		
$C_p^{\circ} =$	272.01		
S° =	208.68		
$\Delta_f S^{\circ} =$	-468.72		
$\Delta_{t}G^{\circ} =$	-262.69		
$lnK_f =$	105.97		
Solid phase			
$\Delta_t H^{\circ} = -383.00$	-408.91	25.91	53SMI/BJE
$C_p^{\circ} =$	151.86		
<i>S</i> ° =	172.04		
$\Delta_f S^\circ =$	- 505.36		
$\Delta_{\mathbf{f}}G^{\circ} =$	-258.24		
$lnK_f =$	104.17		

TABLE 51.	Chlorides ((116) -	Continued
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Chloroacetic acid $C_2H_3ClO_2$ $(1 \times C - (H)_2(CO)(Cl)) + (1 \times CO - (C)(O)) + (1 \times O - (H)(CO))$	2-Chlorobutanoic acid C_4H_7CIO $(1 \times O - (H)(CO)) + (1 \times CO - (C)(O)) + (1 \times C - (H)_2(CO)(Cl)) +$ $(1 \times C - (H)_2(C)_2) + (1 \times C - (H)_3(C))$
Literature - Calculated = Residual Reference	Literature – Calculated = Residual Reference
Gas phase $\Delta_t H^\circ = -435.20 -435.80 0.60 49SRE/MAR$	Gas phase $\Delta_t H^{\alpha} = -498.69$
Liquid phase $\Delta_i H^\circ = -493.42$	Liquid phase $\Delta_t H^\circ = -575.50 - 566.76 - 8.74$ 53SMI/BJE
Solid phase $\Delta_i H^\circ = -510.50 -510.50$ 0.00 53SMI/BJE	Solid phase $\Delta_t H^\circ = -586.65$
2-Chloropropanoic acid $C_3H_5ClO_2$ $(1 \times O-(H)(CO)) + (1 \times CO-(C)(O)) + (1 \times C-(H)_3(C)) +$ $(1 \times C-(H)(C)(CO)(Cl))$ Literature — Calculated = Residual Reference	3-Chlorobutanoic acid $ (1 \times O - (H)(CO)) + (1 \times CO - (C)(O)) + (1 \times C - (H)_2(CO)(C)) + (1 \times C - (H)(C)_2(CI)) + (1 \times C - (H)_3(C)) $ Literature – Calculated = Residual Reference
Gas phase $\Delta_t H^\circ = -473.68$	Gas phase $\Delta_t H^{\circ} = -511.25$ $C_P^{\circ} = 126.21$
Liquid phase $\Delta_{\rm p}H^{\circ} = -522.50 - 518.08 -4.42$ 53SMI/BJE $C_p^{\circ} = 168.73$	Liquid phase $\Delta_t H^\circ = -556.30 -577.93$ 21.63 53SMI/BJE $C_p^\circ = 214.59$
3-Chloropropanoic acid $C_3H_5ClO_2$ $(1\times O-(H)(CO))+(1\times CO-(C)(O))+(1\times C-(H)_2(CO)(C))+$ $(1\times C-(H)_2(C)(Cl))$ Literature – Calculated – Residual Reference	4-Chlorobutanoic acid $C_4H_7ClO_2$ $(1 \times O - (H)(CO)) + (1 \times CO - (C)(O)) + (1 \times C - (H)_2(CO)(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)(Cl))$
Gas phase $\Delta_l II^{\circ}482.83$ $C_{\rho}^{\circ} = 103.01$	Literature - Calculated = Residual Reference Gas phase
Liquid phase $\Delta_t H^o = -546.05$	$\Delta_{i}H^{\circ} = -503.46$ $C_{P}^{\circ} = 125.90$
$C_{\rho}^{\alpha} = 175.85$ $S^{\alpha} = 215.14$ $\Delta_{f}S^{\alpha} = -445.04$ $\Delta_{f}G^{\alpha} = -413.36$ $\ln K_{f} = 166.75$	Liquid phase $\Delta_t H^\circ = -566.30 -571.78$ 5.48 53SMI/BJE $C_p^\circ = 206.27$ $S^\circ = 247.52$ $\Delta_t S^\circ = -548.97$
Solid phase $\Delta_t H^\circ = -549.30 - 549.30 0.00 53SMI/BJE$	$\Delta_{\ell}G^{\circ} = -408.11$ $\ln K_{\ell} = 164.63$

Reference

53SMI/BJE

Dichloroacetic acid

Gas phase $\Delta_{\rm f}H^{\circ} =$

Liquid phase $\Delta_{i}H^{\circ} = -496.30$

2-Chlorobenzoic acid

TABLE 51. Chlorides (116) - Continued

 $(1 \times O-(H)(CO)) + (1 \times CO-(C)(O)) + (1 \times C-(H)(CO)(CI)_2)$

Literature - Calculated = Residual

-431.94

-490.12

 $(4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (Cl)(C_B)_2) + (1 \times O - (H)(CO)) +$

 $(1 \times CO-(O)(C_B)) + (1 \times C_B-(CO)(C_B)_2) +$

(1×ortho corr-(Cl)(COOH))

-6.18

TABLE 51. Chlorides (116) - Continued C₂H₂Cl₂O₂ 4-Chlorobenzoic acid C7H5ClO2 $(4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (Cl)(C_B)_2) + (1 \times O - (H)(CO)) +$ $(1 \times CO-(O)(C_B)) + (1 \times C_B-(CO)(C_B)_2)$ Literature - Calculated = Residual Reference Gas phase $\Delta_t H^{\circ} = -341.00$ -325.59-15.4138WOL/WEG Liquid phase $\Delta_t H^\circ =$ -414.70 $C_p^{\circ} =$ 216.36 C7H5ClO2 Solid phase $\Delta_{\rm f}H^{\circ} =$ -428.16-424.88 -3.2874JOH/PRO $C_p^{\circ} = S^{\circ} =$ 159.53 188.36 $\Delta_f S^{\circ} =$ -494.78 $\Delta_t G^{\circ} =$ -277.36 $lnK_f =$ 111.89 2-Chlorobenzaldehyde C7H5ClO $(4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (CO)(C_B)_2) + (1 \times C_B - (CI)(C_B)_2) +$ $(1 \times CO-(H)(C_B)) + (1 \times ortho corr-(Cl)(CHO))$ Literature - Calculated = Residual Reference Gas phase $\Delta_f H^{\circ} =$ -62.70-74.3911.69 49DRE/MAR Liquid phase $\Delta_{\rm f} H^{\circ} =$ 53SMI/BJE -118.40-118.680.28 $C_p^{\circ} =$ 184.60 3-Chlorobenzaldehyde C7H5ClO $(4 \times C_{B}-(H)(C_{B})_{2}) + (1 \times C_{B}-(CI)(C_{B})_{2}) + (1 \times C_{B}-(CO)(C_{B})_{2}) +$ $(1 \times CO-(H)(C_B))$ Literature - Calculated = Residual Reference Gas phase $\Delta_f H^\circ =$ -67.64Liquid phase $\Delta_i H^\circ =$ -125.90-127.181.28 53SMI/BJE $C_p^{\circ} =$ 184.60

Literatu	re – Calculated	= Residual	Reference
Gas phase			
$\Delta_i H^{\circ} = -325.00$	- 325.59	0.59	38WOL/WEC
Liquid phase			
$\Delta dH^{\circ} =$	- 414.70		
$C_p^{\circ} =$	216.36		
Solid phase			
$\Delta_t H^\circ = -404.83$	- 404.88	0.05	74JOH/PRO
$C_p^{\circ} =$	159.53	2.00	
S° =	188.36		
$\Delta_{i}S^{\circ} =$	- 494.78		
$\Delta_{\rm f}G^{\circ} =$	-257.36		
$\ln K_{\rm f} =$	103.82		
3-Chlorobenzoic acid (4×C _B -(H)(C _B) ₂)+ (1×CO-(O)(C _B))+			C ₇ H ₅ Cl ⁶ (H)(CO))+
3-Chlorobenzoic acid (4×C _B -(H)(C _B) ₂)+ (1×CO-(O)(C _B))+		$(C_B)_2$	
3-Chlorobenzoic acid (4×C _B -(H)(C _B) ₂)+ (1×CO-(O)(C _B))+ Literate	$+(1\times C_{B}-(CO))$	$(C_B)_2$	(H)(CO))+
3-Chlorobenzoic acid (4×C _B -(H)(C _B) ₂)+ (1×CO-(O)(C _B))+	$+(1\times C_{B}-(CO))$	$(C_B)_2$	(H)(CO))+
3-Chlorobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + Literatu$ Gas phase $\Delta_t H^\circ = -342.30$	+ (1 × C _B -(CO)(ure – Calculated	C _B) ₂) = Residual	(H)(CO))+ Reference
3-Chlorobenzoic acid (4×C _B -(H)(C _B) ₂)+ (1×CO-(O)(C _B))+ Literate Gas phase	+ (1 × C _B -(CO)(ure – Calculated	C _B) ₂) = Residual	(H)(CO))+ Reference
3-Chlorobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + Literatu$ Gas phase $\Delta_t H^\circ = -342.30$ Liquid phase	+ (1 × C _B -(CO)(ure – Calculated – 325.59	C _B) ₂) = Residual	(H)(CO))+ Reference
3-Chlorobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + Literatu$ Gas phase $\Delta_t H^\circ = -342.30$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$	+ (1 × C _B -(CO)) ure - Calculated - 325.59 - 414.70	C _B) ₂) = Residual	(H)(CO))+ Reference
3-Chlorobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + Literatu$ Cas phase $\Delta_t H^\circ = -342.30$ Liquid phase $\Delta_t H^\circ = -442.30$	+ (1 × C _B -(CO)) ure - Calculated - 325.59 - 414.70	C _B) ₂) = Residual	(H)(CO))+ Reference
3-Chlorobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + Literatu$ Cas phase $\Delta_t H^\circ = -342.30$ Liquid phase $\Delta_t H^\circ = C_p^\circ = -342.30$ Solid phase $\Delta_t H^\circ = -424.59$	- 325.59 - 414.70 216.36	C _B) ₂) = Residual - 16.71	(H)(CO)) + Reference 38WOI /WEC
3-Chlorobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + Literatu$ Gas phase $\Delta_t H^\circ = -342.30$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ Solid phase	- 325.59 - 414.70 216.36	C _B) ₂) = Residual - 16.71	(H)(CO)) + Reference 38WOI /WEC
3-Chlorobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + Literatu$ Cas phase $\Delta_t H^\circ = -342.30$ Liquid phase $\Delta_t H^\circ = C_\rho^\circ = -342.30$ Solid phase $\Delta_t H^\circ = -424.59$ $C_\rho^\circ = -424.59$ $C_\rho^\circ = -424.59$	- 325.59 - 414.70 216.36 - 424.88 159.53	C _B) ₂) = Residual - 16.71	(H)(CO)) + Reference 38WOI /WEC
3-Chlorobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + Literatu$ Gas phase $\Delta_t H^\circ = -342.30$ Liquid phase $\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -424.59$ $C_p^\circ = S^\circ =$	- 325.59 - 414.70 216.36 - 424.88 159.53 188.36	C _B) ₂) = Residual - 16.71	(H)(CO)) + Reference 38WOI /WEC

Literature - Calculated						
	l = Residual	Reference	Liter	rature – Calculated	l = Residual	Reference
Sas phase Δ _t H° = -67.64			Liquid phase $ \Delta_t H^\circ = -335.6 $ $ C_\rho^\circ = S^\circ = $	0 – 316.94 191.79 279.53	- 18.66	67FAI/STI
Liquid phase $\Delta_t H^\circ = -127.18$ $C_p^\circ = 184.60$			$\Delta_t S^\circ = \Delta_t G^\circ = In K_t =$	- 545.01 - 154.45 62.30		
Solid phase $\Delta_p H^\circ = -146.40 - 157.91$	11.51	53SMI/BJE		te + (1 × C-(H) ₂ (C) ₂)) + (1 × CO-(C)(O		
,2,3-Trichlorobutanal (1×C-(H) ₃ (C))+(1×C-(H)(C) ₂ ((1×CO-(H)(C))	Cl))+(1×C-(0	C ₄ H ₅ Cl ₃ O C) ₂ (Cl) ₂) +		rature – Calculated		Reference
Literature – Calculate	d = Residual	Reference	Gas phase $\Delta_t H^\circ = -467.0$	0 -466.16	-0.84	70COX/PIL
Gas phase $\Delta_t H^\circ = -301.82$ $C_p^\circ = 144.13$			Liquid phase $\Delta_t H^\circ = -515.6$	0 -512.94	-2.66	54BJE/SMI
Liquid phase $\Delta_t H^\circ = -363.00$ $C_p^\circ = 241.84$ 241.84	0.00	1881REI 	$(1 \times O - (C)(CO))$	+ (2 × C-(H) ₂ (C) ₂)) + (1 × CO-(C)(O)))+(1×C-(H)	₂ (CO)(CI))
C-Chloroethyl vinyl ether $(1 \times C - (H)_2(C)(C1)) + (1 \times C - (H)_2(1 \times C_d - (D)(H)) + (1 \times C_d - (H)_2)$	(O)(C))+(1×0	C ₄ H ₇ ClO)-(C)(C _d))+	Gas phase $\Delta_t H^{\circ} = -487.4$	ature - Calculated	-0.61	Reference 70COX/PIL
Literature Calculate	d = Residual	Reference	Liquid phase			
Gas phase	-1.06	81TRO/NED	$\Delta_t H^\circ = -538.4$	0 -538.67	0.27	54BJE/SMI
$\Delta_t H^{\circ} = -170.10 - 169.04$			Ethyl 2-chloroprop	anoate	10)(0)) . (1	C ₅ H ₉ Clo CO-(C)(O))+
Liquid phase $\Delta_t H^\circ = -208.20 -203.62$	-4.58	81TRO/NED	$(2 \times C - (H)_3(C))$ $(1 \times O - (C)(CO))$	$+ (1 \times C - (H)(C)(C) + (1 \times C - (H)_2(O))$	(C))	
Liquid phase	-4.58	81TRO/NED	(1×0-(C)(CO)	+ (1 × C-(H)(C)(C	(C))	Reference
iquid phase $\Delta_t H^{\circ} = -208.20 -203.62$		C,H,CIO	(1×0-(C)(CO)	+ (1 × C-(H)(C)(C) + (1 × C-(H) ₂ (O)	(C))	

TABLE 51. Chlorides (116) - Continued

Propyl 3-chloropropanoate $ (1 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_2(C)_2) + (1 \times C - (H)_2(C)_2(C)_2(C)_2) + (1 \times C - (H)_2(C)_2(C)_2(C)_2) + (1 \times C - (H)_2(C)_2(C)_2(C)_2(C)_2(C)_2(C)_2(C)_2(C$			H ₁₃ ClO ₂)))+
Literature – Calculated = Residual	Reference	Literature - Calculated = Residual Referen	ice
Gas phase $\Delta_t H^\circ = -485.70 -513.19$ 27.49 $C_p^\circ = 167.53$	70COX/PIL	Gas phase $\Delta_t H^\circ = -502.30 -533.82$ 31.52 70COX/ $C_\rho^\circ = 190.42$	/PIL
Liquid phase $ \Delta_t H^\circ = -537.60 -565.57 27.97 $ $ C_0^\circ - 258.15 $ $ S^\circ = 363.41 $ $ \Delta_t S^\circ = -705.70 $ $ \Delta_t G^\circ = -355.17 $ $ \ln K_t = 143.27 $	53SMI/BJE	Liquid phase $ \Delta_t H^\circ = -557.90 -591.30 33.40 53SMI/I $ $ C^\rho_{\rho} = 288.57 $ $ S^\circ = 395.79 $ $ \Delta_t S^\circ = -809.63 $ $ \Delta_t G^\circ = -349.91 $ $ \ln K_f = 141.15 $	вје
Ethyl 4-chlorobutanoate $(1 \times C - (H)_2(C)(C1)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (1 \times C) - (C)(C)) + (1 \times C) + (1 $		Propyl 2-chlorobutanoate C_{7} I $(2 \times C - (H)_3(C)) + (2 \times C - (H)_2(C)_2) + (1 \times C - (H)(C)(CO)(CI)_2) + (1 \times CO - (C)(O)) + (1 \times O - (C)(CO)) + (1 \times C - (H)_2(O)(C))$ Literature – Calculated = Residual Referen	
Gas phase $\Delta_t H^\circ = -513.80 -513.19 -0.61$ $C_p^\circ = 167.53$	70COX/PIL	Gas phase $\Delta_t H^\circ = -578.40 -524.67 -53.73 70COX/$	PIL
Liquid phase $\Delta_t H^\circ = -566.50565.57 - 0.93$	53SMI/BJE	Liquid phase $\Delta_t H^{\circ} = -630.70 -563.33 -67.37$ 53SMI/E $C_p^{\circ} = 281.45$	3JE
$C_p^{\circ} = 258.15$ $S^{\circ} = 363.41$ $\Delta_f S^{\circ} = -705.70$ $\Delta_f G^{\circ} = -355.17$ $\ln K_f = 143.27$		Propyl 4-chlorobutanoate C_7H $(1 \times C - (H)_2(C)(Cl)) + (2 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(CO)(C)_2) + (1 \times C - (H)_2(O)(C)) + (1 \times C - (H)_2(O)(C)) + (1 \times C - (H)_2(C))(C) + (1 \times C - (H)_2(C$	H ₁₃ ClO ₂)) +
Butyl 2-chloropropanoate	C ₇ H ₁₃ ClO ₂	Literature – Calculated = Residual Referen	ce
$(1 \times C - (H)(C)(CO)(CI)) + (2 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)(CO)) + (1 \times C - (H)_2(C)(C)) + (2 \times C - (H)_2(C)(C)(C)) + (2 \times C - (H)_2(C)(C)(C)) + (2 \times C - (H)_2(C)(C)(C)) + (2 \times C - (H)_2(C)(C)(C)(C)) + (2 \times C - (H)_2(C)(C)(C)(C)(C)) + (2 \times C - (H)_2(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)($		Gas phase $\Delta_i H^\circ = -537.90 -533.82 -4.08 70 \text{COX/}$ $C_p^\circ = 190.42$	PIL
Gas phase $\Delta_t H^\circ = -517.40 -524.67$ 7.27	70COX/PIL	Liquid phase $\Delta_t H^\circ = -591.40 -591.30 -0.10$ 53SMI/E $C_p^\circ = 288.57$	вјЕ
Liquid phase $\Delta_i H^{\circ} = -571.70 -563.33 -8.37$ $C_p^{\circ} = 281.45$	53SMI/BJE	$S^{\circ} = 395.79$ $\Delta_{t}S^{\circ} = -809.63$ $\Delta_{t}G^{\circ} = -349.91$ $\ln K_{t} = 141.15$	

TABLE 51. Chlorides (116) - Continued

			(CO)(Cl))+ (C))+(1×C-((1 × CO−(C)(O)) + H)₃(C))				+ (1 × C-(H)()) + (1 × C-(H)	C)(CO)(CI))+ ₂ (O)(C))
	Literature	- Calculated	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas phase Δ _t H° =		-510.60			Liquid phase $\Delta_t H^\circ = -C_p^\circ =$: - 655.30	- 589.06 311.87	- 66.24	53SMI/BJE
Liquid phase $\Delta_t H^\circ = C_p^\circ =$	248.95	-551.16 247.89	1.06	53SMI/BJE		(CO)(Cl) ₂		C)(O))+(1×C C) ₂)+(1×C-(
3-Methylbuty (3×C-(H)			O)(CI))+(1×	C ₈ H ₁₅ ClO ₂ CO–(C)(O))+		Literatur	e – Calculated	= Residual	Reference
)(C) ₃)+(2×	× C-(H) ₂ (O)(CH ₃ corr (t Calculated	• • • • • • • • • • • • • • • • • • • •	H) ₂ (C) ₂) + Reference	Gas phase $\Delta_t H^\circ = -$	- 497.80	-482.93	- 14.87	70COX/PIL
Gas phase Δ _ℓ H° = -	- 575.00	-551.99	-23.01	70COX/PIL	Liquid phase $\Delta_t H^\circ = -$		-535.37	-14.73	53SMI/BJE
•	e 627.30	- 594.34 308.89	- 32.96	53SMI/BJE	2-Methylprop (1×C-(H)	(CO)(CI) ₂)+(1×CO-(0	C)(O))+(1×C C) ₃)+(2×C-(F	C ₆ H ₁₀ Cl ₂ O >-(C)(CO)) + {}\ ₂ (C)) +
C _p =					(2×-CH₃			73) 1 (21.0 (1	-/3(-//
3-Methylbuty	yl 3-chlorop			C ₈ H ₁₅ ClO ₂		corr (tertia			Reference
3-Methylbuty (1 × C-(H) (1 × O-(C)) ₂ (C)(Cl))+ ()(CO))+(1	ropanoate (1×C-(H) ₂ (0) ×C-(H) ₂ (O)(CO)(C))+(1× C))+(1×C-(+(2×-CH ₃ co	(CO-(C)(O))+ H) ₂ (C) ₂)+	(2×-CH ₃	corr (tertia	ary))		
3-Methylbuty (1 × C-(H) (1 × O-(C)) ₂ (C)(Cl))+ ()(CO))+(1 ()(C) ₃)+(2×	ropanoate (1×C-(H) ₂ (0) ×C-(H) ₂ (O)((C)) + $(1 \times C - (C)$ + $(2 \times - CH_3)$ co	(CO-(C)(O))+ H) ₂ (C) ₂)+	$(2 \times \text{-CH}_3)$ Gas phase $\Delta_1 H^\circ = -$ Liquid phase	Literatur	ary)) e – Calculated	= Residual	Reference
3-Methylbuty (1 × C-(H) (1 × O-(C) (1 × C-(H))) ₂ (C)(Cl))+ ()(CO))+(1 ()(C) ₃)+(2×	ropanoate · (1 × C-(H) ₂ (0) × C-(H) ₃ (C)) -	(C)) + $(1 \times C - (C)$ + $(2 \times - CH_3)$ co	$(CO-(C)(O)) + H)_2(C)_2) + $ or (tertiary))	$(2 \times \text{-CH}_3)$ Gas phase $\Delta_t H^\circ = -$	Literatur	ary)) e – Calculated	= Residual	Reference
3-Methylbuty $(1 \times C - (H))$ $(1 \times C - (H))$ $(1 \times C - (H))$ Gas phase $\Delta_t H^\circ = C_\rho^\circ =$ Liquid phase $\Delta_t H^\circ = C_\rho^\circ = C_$) ₂ (C)(Cl)) + (1 c)(CO)) + (1 c)(C) ₂) + (2 × Literature - 539.40	ropanoate (1 × C-(H) ₂ (O)(× C-(H) ₃ (C)) - - Calculated -561.14 213.34 -622.31	$\begin{array}{l} (C)) + (1 \times C - (1 \times C - (1 \times C - C)) \\ + (2 \times - CH_3) \\ = \text{Residual} \end{array}$	CCO-(C)(O)) + H) ₂ (C) ₂) + or (tertiary)) Reference	Gas phase $\Delta_{l}H^{\circ} = -$ Liquid phase $\Delta_{l}H^{\circ} = -$ 3-Methylbuty $(1 \times C - (H))$ $(1 \times C - (H))$	Literature - 501.50 - 553.80 - I dichloros (CO)(Cl) ₂ ₂ (O)(C)) +	e – Calculated – 489.62 – 540.65 acetate) + (1 × CO-(0	= Residual -11.88 -13.15 C)(O)) + (1 × O)(C) ₂) + (1 × C-(1)(C) ₂)	Reference 70COX/PIL 53SMI/BJE C ₇ H ₁₂ Cl ₂ O ₅ (C)(CO)) +
3-Methylbuty $(1 \times C - (H))$ $(1 \times C - (H))$ $(1 \times C - (H))$ Gas phase $\Delta_t H^{\circ} = -C_{\rho}^{\circ} =$ Liquid phase $\Delta_t H^{\circ} = -C_{\rho}^{\circ} = -C_{\rho}^{\circ}$) ₂ (C)(Cl)) + (1 c)(CO)) + (1 c)(C) ₂) + (2 × Literature - 539.40	ropanoate (1 × C-(H) ₂ (O)(× C-(H) ₃ (C)) - - Calculated - 561.14 213.34 - 622.31 316.01 422.82	(C)) + $(1 \times C - (1 \times C - (1 \times C - CH_3 \cos CH_3 \cos$	CCO-(C)(O)) + H) ₂ (C) ₂) + orr (tertiary)) Reference	Gas phase $\Delta_{l}H^{\circ} = -$ Liquid phase $\Delta_{l}H^{\circ} = -$ 3-Methylbuty $(1 \times C - (H))$ $(1 \times C - (H))$	Literature - 501.50 - 553.80 I dichloros (CO)(Cl) ₂ ₂ (O)(C)) + (23)	e – Calculated - 489.62 - 540.65 acetate) + (1 × CO – (0 – (1 × C – (H) ₂ (0	= Residual - 11.88 - 13.15 C)(O)) + (1 × O C) ₂) + (1 × C-(1) ertiary))	Reference 70COX/PIL 53SMI/BJE C ₇ H ₁₂ Cl ₂ O ₅ (C)(CO)) +
3-Methylbuty $(1 \times C - (H))$ $(1 \times C - (H))$ $(1 \times C - (H))$ Gas phase $\Delta_t H^{\circ} = -C_p^{\circ} =$ Liquid phase $\Delta_t H^{\circ} = -C_p^{\circ} $) ₂ (C)(Cl)) + (1 c)(CO)) + (1 c)(C) ₂) + (2 × Literature - 539.40	ropanoate (1×C-(H) ₂ (O)(×C-(H) ₃ (C)) - - Calculated -561.14 213.34 -622.31 316.01	(C)) + $(1 \times C - (1 \times C - (1 \times C - CH_3 \cos CH_3 \cos$	CCO-(C)(O)) + H) ₂ (C) ₂) + orr (tertiary)) Reference	Gas phase $\Delta_t H^\circ = -$ Liquid phase $\Delta_t H^\circ = -$ 3-Methylbuty $(1 \times C - (H))$ $(1 \times C - (H))$ $(2 \times C - (H))$ Gas phase	Literature - 501.50 - 553.80 I dichloros (CO)(Cl) ₂ ₂ (O)(C)) + (23)	= - Calculated - 489.62 - 540.65 acetate) + (1 × CO-(C-(1 × C-(H) ₂)(C-(X - CH ₃ corr (6)	= Residual - 11.88 - 13.15 C)(O)) + (1 × O C) ₂) + (1 × C-(1) ertiary))	Reference 70COX/PIL 53SMI/BJE C ₇ H ₁₂ Cl ₂ O ₂ (-(C)(CO)) + H)(C) ₃) +
3-Methylbuty $(1 \times C - (H))$ $(1 \times C - (H))$ $(1 \times C - (H))$ Gas phase $\Delta_t H^\circ = -C_\rho^\circ =$ $Liquid phase$ $\Delta_t H^\circ = -C_\rho^\circ =$ $S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = inK_t =$ Butyl 2-chlor $(2 \times C - (H))$	- 539.40 cobutanoate - (3) cobutanoate - (3) cobutanoate - (3)	ropanoate (1 × C-(H) ₂ (O) ₀ × C-(H) ₃ (O))- - Calculated - 561.14 213.34 - 622.31 316.01 422.82 - 918.91 - 348.34 140.52	(C)) + (1 × C-(+ (2 × -CH ₃ co = Residual 21.74 28.91	CCO-(C)(O)) + H) ₂ (C) ₂) + orr (tertiary)) Reference 70COX/PIL 53SMI/BJE C ₈ H ₁₅ ClO ₂ C)(CO)(Cl)) +	Gas phase $\Delta_{t}H^{\circ} = -$ Liquid phase $\Delta_{t}H^{\circ} = -$ 3-Methylbuty $(1 \times C - (H))$ $(1 \times C - (H))$ $(2 \times C - (H))$ Gas phase $\Delta_{t}H^{\circ} = -$ Liquid phase	Literature - 501.50 - 553.80 - 1 dichloros (CO)(Cl) ₂ ₂ (O)(C)) + (2) Literature	ary)) e - Calculated - 489.62 - 540.65 acetate)+(1 × CO-(C (1 × C-(H) ₂ (C × -CH ₃ corr (t) e - Calculated	= Residual -11.88 -13.15 $C(O) + (1 \times O)$ $C(C)_2 + (1 \times C - O)$ ertiary)	Reference 70COX/PIL 53SMI/BJE C ₇ H ₁₂ Cl ₂ O ₂ (C)(CO)) + H)(C) ₃) + Reference
3-Methylbuty $(1 \times C - (H))$ $(1 \times C - (H))$ $(1 \times C - (H))$ Gas phase $\Delta_t H^\circ = -C_\rho^\circ =$ $Liquid phase$ $\Delta_t H^\circ = -C_\rho^\circ =$ $S^\circ = \Delta_t S^\circ = \Delta_t S^\circ = inK_t =$ Butyl 2-chlor $(2 \times C - (H))$	- 539.40 robutanoate 3(C)(C)()) + (1)(C)(1) + (2) 4(2)(C)(1) + (2)(2) 539.40 539.40 6	ropanoate (1 × C-(H) ₂ (O) ₀ × C-(H) ₃ (O))- - Calculated - 561.14 213.34 - 622.31 316.01 422.82 - 918.91 - 348.34 140.52	$(C) + (1 \times C - (C)) + (1 \times C - (C)) + (1 \times C - (C)) + (2 \times - CH_3) + (21.74)$ 21.74 28.91 $+ (1 \times C - (H)(C)) + (1 \times C - (H)(C)) + (1 \times C - (H)(C))$	CCO-(C)(O)) + H) ₂ (C) ₂) + orr (tertiary)) Reference 70COX/PIL 53SMI/BJE C ₈ H ₁₅ ClO ₂ C)(CO)(Cl)) +	Gas phase $\Delta_{t}H^{\circ} = -$ Liquid phase $\Delta_{t}H^{\circ} = -$ 3-Methylbuty $(1 \times C - (H))$ $(1 \times C - (H))$ $(2 \times C - (H))$ Gas phase $\Delta_{t}H^{\circ} = -$ Liquid phase	Literature - 501.50 - 553.80 - 1 dichloros (CO)(Cl) ₂ ₂ (O)(C)) + (2) Literature	ary)) e - Calculated - 489.62 - 540.65 acetate) + (1 × CO-(C) - (1 × C-(H) ₂ (C) × - CH ₃ corr (t) e - Calculated	= Residual - 11.88 - 13.15 C)(O)) + (1 × O(C) ₂) + (1 × C-(1) ertiary)) = Residual - 9.15	Reference 70COX/PIL 53SMI/BJE C ₇ H ₁₂ Cl ₂ O ₂ (CO)(CO)) + H)(C) ₃) + Reference

TABLE 51. Chlorides (1	116) —	Continued
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		1. Chlorides (1	-0, Will	
Pentanoyl c		WC (II) (C))	. (1 × C (II) /	C ₅ H ₉ ClO
(1×C-(F		\times C-(H) ₂ (C) ₂) -	+(1 × C−(H) ₂ ((CO)(C))+
	Literatu	re – Calculated :	= Residual	Reference
Gas phase				
$\Delta_{\mathbf{f}}H^{\circ} = C_{p}^{\circ} =$		-305.90 138.29		
Liquid phas	se			
$\Delta_l H^\circ = C_p^\circ =$	197 96	-348.50	10.42	1001DET
	187.86	207.28	- 19.42 	1881REI
2-Methylpro	opanoyl chi	loride		C ₄ H ₇ Cl0
(2×C-(I		×C-(H)(CO)(C) ₂)+(1×CO	
	Literatu	re – Calculated =	= Residual	Reference
Gas phase				
$\Delta_{\rm f}H^{\circ} =$		- 289.83		
Liquid phas	se			
$\Delta_t H^\circ = C_\rho^\circ =$	131.80	- 328.76 171.04	- 39.24	1881REI
——————————————————————————————————————		171.04		
Benzoyl chl				C7H5(
(5 × C _B ~((1×C _B -(CO)(C		
	Literatu	re – Calculated =	= Kisiduai	Reference
Liquid phas $\Delta_t H^\circ =$	se	- 165.37		
$C_p^{\circ} =$	187.00	187.00	0.00	1881REI
Chioroacety (1×CO-		(1×C-(H) ₂ (CO))(Cl))	C ₂ H ₂ Cl ₂ (
	Literatu	re – Calculated =	= Residual	Reference
Gas phase				
$\Delta_t H^{\circ} =$	-244.80	-244.80	0.00	70COX/PIL
Liquid phas		-283.70	0.00	50PRI/SKI

cetyl chlori (1×C-(H		1×CO-(C)(Cl)), $\sigma = 3$	C₂H₃ClO
	Literatur	Reference		
Gas phase				
-	- 242.70	-242.80	0.10	31MAT/FEH
	67.82	67.82	0.00	69STU/WES
S° =	294.85	294.85	0.00	69STU/WES
$\Delta_f S^\circ =$	27	- 126.50	0.00	5.51.5, <u>-</u> 2.
$\Delta_{\rm f}G^{\circ} =$		- 205.08		
$\ln K_f =$		82.73		
Liquid phas		272.00	0.10	ADC A D /CIZI
$\Delta_i H^\circ = C_p^\circ =$	-2/2.80 117.15	-272.90	0.10	49CAR/SKI
C _p =	117.15	117.15	0.00	1881REI
	etyl chlorid			C₂HCl₃C
(1×C-(I	1)(CO)(Cl)	2)+(1×CO-(C))(Cl))	
	Literatu	re – Calculated =	= Residual	Reference
Gas phase				
-	-241.00	- 240.94	-0.06	70COX/PIL
· · · · · · · · · · · · · · · · · · ·				
Liquid phas $\Delta_t H^\circ =$ Propanoyl	- 280.40 chloride	-280.40	0.00	
$\Delta_i H^\circ =$ Propancyl	-280.40 chloride H) ₃ (C))+(1	× C-(H)₂(CO)((C))+(1×CO	C₃H₅ClO ⊢(C)(Cl))
Δ _i H° =	-280.40 chloride H) ₃ (C))+(1		(C))+(1×CO	C ₃ H ₅ ClO
Δ _t H° = Propancyl (1×C-(I	-280.40 chloride H) ₃ (C))+(1	× C-(H)₂(CO)((C))+(1×CO	C₃H₅Cl(⊢(C)(Cl))
$\Delta_t H^\circ =$ Propancyl (1×C-(F)) Gas phase	-280.40 chloride H) ₃ (C))+(1	×C-(H) ₂ (CO)(re – Calculated	(C))+(1×CO	C₃H₅Cl(⊢(C)(Cl))
Δ _t H° = Propancyl (1×C-(I	-280.40 chloride H) ₃ (C))+(1	× C-(H)₂(CO)((C))+(1×CO	C₃H₅Cl(⊢(C)(Cl))
$\Delta_t H^\circ =$ Propancy (1 × C-(1) Gas phase $\Delta_t H^\circ =$	-280.40 chloride H) ₃ (C))+(1	× C-(H) ₂ (CO)(re - Calculated = - 264.64	(C))+(1×CO	C₃H₅Cl(⊢(C)(Cl))
$\Delta_t H^\circ =$ Propancy! $(1 \times C - (I \times C - (I \times C - (I \times C + (I \times C) + (I \times C))))))))))))$	-280.40 chloride H) ₃ (C))+(1 Literatu	× C-(H) ₂ (CO)(re – Calculated : – 264.64 92.51	(C))+(1×CO	C₃H₅Cl(⊢(C)(Cl))
$\Delta_t H^\circ =$ Propanoyi $(1 \times C - (I \times C - (I \times C - (I \times C + (I \times C) + (I \times C) + (I \times C) + (I \times C + (I \times C) + $	-280.40 chloride H) ₃ (C))+(1 Literatu	× C-(H) ₂ (CO)(re - Calculated = - 264.64	(C))+(1×CO	C₃H₅Cl(⊢(C)(Cl))
$\Delta_t H^\circ =$ Propanoyi $(1 \times C - (I \times C)))))))))))))))))$	-280.40 chloride H) ₃ (C))+(1 Literatu	× C-(H) ₂ (CO)(re – Calculated : – 264.64 92.51	(C))+(1×CO	C₃H₅Cl(⊢(C)(Cl))
$\Delta_t H^\circ =$ Propanoyi $(1 \times C - (I \times C - (I \times C - (I \times C + (I \times C) + (I \times C) + (I \times C) + (I \times C + (I \times C) + $	-280.40 chloride H) ₃ (C))+(1 Literatu	× C-(H) ₂ (CO)(re - Calculated = -264.64 92.51	(C)) + (1 × CO = Residual	C₃H₅CIC ⊢(C)(CI)) Reference
Propanoyi (1×C-(H) Gas phase $\Delta_t H^\circ = C_\rho^\circ =$ Liquid pha $\Delta_t H^\circ = C_\rho^\circ =$ Butanoyi ci	280.40 chloride H) ₃ (C)) + (1 Literatu se 147.28	× C-(H) ₂ (CO)(re - Calculated 264.64 92.51 - 297.04 146.44	(C)) + (1 × CO = Residual 0.84	C ₃ H ₅ CIC ⊢(C)(CI)) Reference 1881REI
$\Delta_t H^\circ =$ Propanoyi $(1 \times C - (I \times C - (I \times C - (I \times C + (I \times C$	280.40 chloride H) ₃ (C)) + (1 Literatu se 147.28	× C-(H) ₂ (CO)(re - Calculated = -264.64 92.51	(C)) + (1 × CO = Residual 0.84	C ₃ H ₅ CIC ⊢(C)(CI)) Reference 1881REI
$\Delta_t H^\circ =$ Propanoyi $(1 \times C - (I \times C - (I \times C - (I \times C + (I \times C$	280.40 chloride H) ₃ (C)) + (1 Literatu see 147.28 hloride H) ₃ (C)) + (1 -(C)(Cl))	× C-(H) ₂ (CO)(re - Calculated 264.64 92.51 - 297.04 146.44	(C)) + (1 × CO = Residual 0.84 + (1 × C-(H) ₂)	C ₃ H ₅ CIC ⊢(C)(CI)) Reference 1881REI
$\Delta_t H^\circ =$ Propancy: $(1 \times C - (I \times C - (I \times C - (I \times C + C)))$ Gas phase $\Delta_t H^\circ = C_p^\circ =$ Liquid pha $\Delta_t H^\circ = C_p^\circ =$ Butancy: $(1 \times C - (I \times C - (I \times C)))$	280.40 chloride H) ₃ (C)) + (1 Literatu see 147.28 hloride H) ₃ (C)) + (1 -(C)(Cl))	× C-(H) ₂ (CO)(re - Calculated = -264.64 92.51 -297.04 146.44	(C)) + (1 × CO = Residual 0.84 + (1 × C-(H) ₂)	C ₃ H ₅ CIO (C)(CI)) Reference 1881REI C ₄ H ₇ CIO (CO)(C)) +
$\Delta_t H^\circ =$ Propancy: $(1 \times C - (I \times C))))))))))))))))$	280.40 chloride H) ₃ (C)) + (1 Literatu see 147.28 hloride H) ₃ (C)) + (1 -(C)(Cl))	× C-(H) ₂ (CO)(re - Calculated - 264.64 92.51 - 297.04 146.44 l × C-(H) ₂ (C) ₂) are - Calculated	(C)) + (1 × CO = Residual 0.84 + (1 × C-(H) ₂)	C ₃ H ₅ CIO (C)(CI)) Reference 1881REI C ₄ H ₇ CIO (CO)(C)) +
$\Delta_t H^\circ =$ Propancyl (1×C-(H Gas phase $\Delta_t H^\circ =$ $C_\rho^\circ =$ Liquid pha $\Delta_t H^\circ =$ $C_\rho^\circ =$ Butancyl ci (1×C-(I (1×CO-Gas phase $\Delta_t H^\circ =$	280.40 chloride H) ₃ (C)) + (1 Literatu see 147.28 hloride H) ₃ (C)) + (1 -(C)(Cl))	× C-(H) ₂ (CO)(re - Calculated - 264.64 92.51 - 297.04 146.44 l × C-(H) ₂ (C) ₂) are - Calculated - 285.27	(C)) + (1 × CO = Residual 0.84 + (1 × C-(H) ₂)	C ₃ H ₅ CIO (CO)(CI)) Reference 1881REI C ₄ H ₇ CIO(CO)(C)) +
$\Delta_t H^\circ =$ Propancy: $(1 \times C - (I \times C))))))))))))))))$	280.40 chloride H) ₃ (C)) + (1 Literatu see 147.28 hloride H) ₃ (C)) + (1 -(C)(Cl))	× C-(H) ₂ (CO)(re - Calculated - 264.64 92.51 - 297.04 146.44 l × C-(H) ₂ (C) ₂) are - Calculated	(C)) + (1 × CO = Residual 0.84 + (1 × C-(H) ₂)	C ₃ H ₅ CIO (CO)(CI)) Reference 1881REI C ₄ H ₇ CIO(CO)(C)) +
$\Delta_t H^\circ =$ Propancyl (1×C-(H Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ Butancyl cl (1×C-(I (1×CO-Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$	280.40 chloride H) ₃ (C)) + (1 Literatu see 147.28 hloride H) ₃ (C)) + (1 -(C)(Cl)) Literatu	× C-(H) ₂ (CO)(re - Calculated - 264.64 92.51 - 297.04 146.44 l × C-(H) ₂ (C) ₂) are - Calculated - 285.27	(C)) + (1 × CO = Residual 0.84 + (1 × C-(H) ₂)	C ₃ H ₅ CIO (C)(CI)) Reference 1881REI C ₄ H ₇ CIO (CO)(C)) +
$\Delta_t H^\circ =$ Propancyl (1×C-(H Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ Butancyl cl (1×C-(I) (1×CO-Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ Liquid pha	280.40 chloride H) ₃ (C)) + (1 Literatu see 147.28 hloride H) ₃ (C)) + (1 -(C)(Cl)) Literatu	× C-(H) ₂ (CO)(re - Calculated - 264.64 92.51 - 297.04 146.44 1 × C-(H) ₂ (C) ₂) are - Calculated - 285.27 115.40	(C)) + (1 × CO = Residual 0.84 + (1 × C-(H) ₂)	C ₃ H ₅ CIO (C)(CI)) Reference 1881REI C ₄ H ₇ CIO (CO)(C)) +
$\Delta_t H^\circ =$ Propancyl (1×C-(H Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$ Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ Butancyl cl (1×C-(I (1×CO-Gas phase $\Delta_t H^\circ =$ $C_p^\circ =$	280.40 chloride H) ₃ (C)) + (1 Literatu see 147.28 hloride H) ₃ (C)) + (1 -(C)(Cl)) Literatu	× C-(H) ₂ (CO)(re - Calculated - 264.64 92.51 - 297.04 146.44 l × C-(H) ₂ (C) ₂) are - Calculated - 285.27	(C)) + (1 × CO = Residual 0.84 + (1 × C-(H) ₂)	C ₃ H ₅ CIO (CO)(CI)) Reference 1881REI C ₄ H ₇ CIO(CO)(C)) +

C₈H₄Cl₂O₂

73SAP/MOC

C₈H₄Cl₂O₂

73SAP/MOC

 $C_p^{\circ} =$

248.50

248.50

0.00

1881REI

TABLE 51. Chlorides (116) - Continued

2-Chlorobenzoyl chloride $(4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (Cl)(C_B)_2) + (1 \times C_{B^{-1}}(Cl)(COCl)) + (1 \times COC - (C_B)(Cl)) + (1 \times OCC)(COCl))$	$C_7H_4Cl_2O$ (CO)(C _B) ₂) +		$-1)(C_B)_2) +$	(2×C _B -(CO)(Cl)(COCl))	$(C_B)_2$ + $(2 \times C_B)_2$	C ₈ H ₄ Cl O-(C _B)(Cl))+
Literature Calculated = Residual	Reference	•	Literatu	re – Calculated	= Residual	Reference
Liquid phase $\Delta_t H^{\circ} = -171.30 -171.30 0.00$ $C_p^{\circ} = 199.59$	75MOS/PRI	Liquid phase $\Delta_t H^\circ = C_p^\circ =$	e	-379.70 237.92		
3-Chlorobenzoyl chloride $(4\times C_B-(H)(C_B)_2)+(1\times C_B-(Cl)(C_B)_2)+(1\times C_{B-(Cl)}(Cl))$ $(1\times CO-(C_B)(Cl))$	$C_7H_4Cl_2O$ (CO)(C _B) ₂)+	Solid phase $\Delta_t H^\circ = -$	- 367.50	-367.50	0.00	73SAP/MOO
Literature – Calculated = Residual	Reference	1,4-Phthaloy (4×C _B -(H		(2×C _B -(CO)(C _B) ₂) + (2 × C0	C ₈ H ₄ Cl ₂ D-(C _B)(Cl))
Liquid phase $\Delta_t H^\circ = -189.70 -205.73$ 16.03 $C_p^\circ = 199.59$	75MOS/PRI		Literatui	e – Calculated	= Residual	Reference
4-Chlorobenzoyl chloride $(4 \times C_R - (H)(C_R)_2) + (1 \times C_R - (Cl)(C_R)_2) + (1 \times C_R - (Cl)(C_$	C ₇ H ₄ Cl ₂ O (CO)(C _B) ₂) +	Liquid phase $\Delta_l H^\circ = C_p^\circ = $ Solid phase		-379.70 237.92		
Literature – Calculated = Residual	Reference	$\Delta_t H^{\circ} = -$	-384.60	-383.56	-1.04	73SAP/MOC
Liquid phase $\Delta_i H^\circ = -191.70 -205.73 $ 14.03 $C_p^\circ = 199.59$	75MOS/PRI					
1,2-Phthaloyl chloride $(4 \times C_B - (H)(C_B)_2) + (2 \times C_B - (CO)(C_B)_2) + (2 \times CO)(1 \times ortho \text{ corr} - (COCl)(COCl))$	$C_8H_4Cl_2O_2$ $\vdash(C_B)(Cl)) +$					
Literature – Calculated = Residual	Reference					

TABLE 52. Bromides (39) — Continue	TABLE	52.	Bromides	(39) -	 Continue
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	I)₃(Br), metl	hyl bromide), o	r = 3		(1×C-(H)₃(C))+(2	$2 \times C - (H)_2(C)_2$	$+(1\times C-(H)_2$	$(C)(Br)), \sigma = 3$
	Literature	e – Calculated =	= Residual	Reference	Literature Calculated = Residual		l = Residual	Reference	
Gas phase					Gas phase				
$\Delta_t H^{\circ} = $	-37.66	-37.66	0.00	38EGA/KEM	$\Delta_{\rm f}H^{\circ} =$	- 107.10	-105.30	-1.80	66WAD2
$C_p^o =$	42.43	42.43	0.00	69STU/WES	$C_p^{\circ} =$	109.33	109.33	0.00	69STU/WE
S° =	245.81	245.81	0.00	69STU/WES	а =	369.82	369.82	0.00	69STU/WE
Δ _t S° =		-31.90			$\Delta_{\rm f} S^{\circ} =$		-316.82		0,010,
$_{i}G^{\circ} =$		-28.15			$\Delta_f G^\circ =$		- 10.84		
$nK_f =$		11.36			$lnK_f =$		4.37		
iquid pha	se				Liquid pha	ase			
idaic biiα VH°=	-61.10	-61.10	0.00	66ADA/CAR	$\Delta_t H^\circ =$	- 143.80	- 141.72	-2.08	61BJE2
·la •	01.10	01.10	0.00	oor idea of the	$C_p^{\circ} =$	152.21	163.32	- 11.11	31DEE
					S° =	132.21	261.06	11.11	JIDEE
					$\Delta_f S^\circ =$		-425.57		
romoetha	200			C ₂ H ₅ Br	$\Delta_{i}G^{\circ} =$		-14.83		
		× C-(H)2(C)(B	r)) ~ - 3	C2115DF	-				
(1×C-(1	<i>/(</i>	()-().	***	5 .	$lnK_f =$		5.98		
	Literatur	e – Calculated	= Residual 	Reference	1-Bromope	entane			C ₅ H ₁
es mb ess					(1×C-($H)_3(C)) + (3$	\times C-(H) ₂ (C) ₂)	$+(1\times C-(H)_2)$	$(C)(Br)), \sigma = 3$
ias phase \aH° =	- 64.02	- 64.04	0.02	69STU/WES		I itamatuu	ra - Calaulat - 4	- Dooldsol	Dafanana-
•						Literatui	re – Calculated	= Residual	Reference
$C_p^{\circ} =$	64.64	63.55	1.09	69STU/WES					
<i>s</i> ° =	287.48	291.50	-4.02	69STU/WES					
Δ _t S° =		- 122.52			Gas phase				
$\Lambda_{\rm f}G^{\circ} =$		- 27.51			$\Delta_t H^{\circ} =$	- 129.10	- 125.93	-3.17	66WAD2
$lnK_f =$		11.10			$C_p^{\circ} =$	132.21	132.22	-0.01	69STU/WE
					S° =	408.78	408.98	-0.20	69STU/WE
					$\Delta_{\mathbf{f}}S^{\circ} =$		-413.97		
iquid pha	ise				$\Delta_f G^{\circ} =$		-2.50		
$\Delta_t H^{\circ} =$	-91.51	- 90.26	- 1.25	69STU/WES	$lnK_f =$		1.01		
$C_p^{\circ} =$	100.80	102,48	- 1.68	48KUR					
S° =		196.30							
$\Delta_f S^\circ =$		-217.71			Liquid pha	ase			
$\Delta_{\mathbf{f}}G^{\circ} =$		-25.35			$\Delta_{\rm f}H^{\circ} =$	- 170.20	- 167.45	-2.75	61BJE2
$lnK_f =$		10.23			$C_p^{\circ} =$	171.59	193.74	-22.15	31DEE
		10.20			S° =	1,1,0,	293.44	22.10	51225
					$\Delta_t S^\circ =$		-529.51		
-Bromopi	ronone			C ₃ H ₂ Br	$\Delta_t G^\circ =$		-9.58		
		\times C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂	$(C)(Br)), \sigma = 3$	$\ln K_{\rm f} =$		3.86		
	Literatu	re – Calculated	= Residual	Reference	-				
					1-Bromoho		\times C-(H) ₂ (C) ₂)	+ (1 × C-(H)-	C ₆ H ₁
Gas phase Δ _I H° =	-87.86	- 84.67	-3.19	69STU/WES	(3)		re – Calculated	, , ,	Reference
$C_p^{\circ} =$	- 87.80 86.44	- 84.07 86.44	0.00	69STU/WES		Liciatul	c – Calculated	- Vesignai	Reference
$S^{\circ} =$									
-	330.87	330.66	0.21	69STU/WES	C !				
$\Delta_f S^\circ =$		-219.67			Gas phase			4	*****
$\Delta_t G^\circ =$		- 19.18			$\Delta_t H^\circ =$	- 148.10	- 146.56	- 1.54	68WAD
		7.74			$C_p^{\circ} =$		155.11		
$lnK_f =$					Liquid pha	ase			
lnK _f =	ase			GGWADO	$\Delta_t H^\circ =$	- 194.20	- 193.18	-1.02	61BJE2
$lnK_{f} =$ Liquid pha	ase 119.76	- 115.99	-3.77	00WADZ					
$lnK_f =$ $Liquid pha$ $\Delta_f H^\circ =$	-119.76			66WAD2 1881REI		203.55	224 16	- 20.61	31DEE
$lnK_f =$ Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$		132.90	-3.77 -2.40	1881REI	$C_p^{\circ} =$	203.55 452.92	224.16 325.82	- 20.61 127.10	31DEE 31DEE
$lnK_f =$ Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$	-119.76	132.90 228.68			$C_p^{\circ} = S^{\circ} =$	203.55 452.92	325.82	- 20.61 127.10	31DEE 31DEE
$lnK_f =$ Liquid pha $\Delta_f H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_f S^\circ =$	-119.76	132.90 228.68 -321.64			$C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = 0$		325.82 -633.44		
$lnK_f =$ $\begin{array}{ccc} & & & \\ &$	-119.76	132.90 228.68			$C_p^{\circ} = S^{\circ} =$		325.82		

TABLE 52. Bromides (39) - Continued

1-Bromohe (1 × C-(1		× C-(H) ₂ (C) ₂) -	+ (1×C-(H) ₂	$C_7H_{15}Br$ (C)(Br))	1-Bromohexadecane (1×C-(H) ₃ (C))+	e - (14 × C-(H) ₂ (C) ₂))+(1×C-(H)	$C_{16}H_{33}B_{2}(C)(Br))$
	Literatur	e – Calculated =	= Residual	Reference	Litera	nture – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 167.70	- 167.19 178.00	-0.51	68WAD	Gas phase $\Delta_t H^\circ = -350.10$ $C_p^\circ =$	- 352.86 384.01	2.76	76STR3
Liquid pha $\Delta_t H^\circ = C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	ase - 218.40	-218.91 254.58 358.20 -737.37 0.94	0.51	61BJE2	Liquid phase $ \Delta_t H^\circ = -444.50 $ $ C_\rho^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \Delta_t G^\circ = 0 $	528.36 649.62 - 1672.75 48.25	5.98	76STR3
$lnK_f =$ 1-Bromood		-0.38	1 (1 × C (B)	C ₈ H ₁₇ Br	$\ln K_{\rm f} = \frac{1 - \text{Bromo-3-methylbr}}{(2 \times C/V)/(C)}$		1 (1 × C (II))	C ₅ H ₁₁ I
(1×C-(× C-(H) ₂ (C) ₂) - e – Calculated = 		Reference	(2×-CH₃ corr (to	· (1 × C-(H) ₂ (C) ₂) - ertiary)) + (1 × C-(ture – Calculated =	H) ₂ (C)(Br))	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	- 189.30	-187.82 200.89	-1.48	77MAN/SEL	Gas phase $\Delta_t H^\circ = C_p^\circ =$	-132.62 132.25		
Liquid pha $\Delta_t H^\circ =$ $C_p^\circ =$ $S^\circ =$ $\Delta_t S^\circ =$ $\Delta_t G^\circ =$ $\ln K_t =$	ase - 245.10	-244.64 285.00 390.58 -841.30 6.19 -2.50	-0.46	61BJE2	Liquid phase $ \Delta_t H^\circ = C_p^\circ = 187.00 $ $ S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	- 172.73 190.76 288.09 - 534.86 - 13.26 5.35	-3.76	48KUR
1-Bromodo (1 × C-(H) ₃ (C))+(10) × C-(H) ₂ (C) ₂) e – Calculated =	, , ,	$C_{12}H_{25}Br$ $_{2}(C)(Br))$ Reference	1-Bromo-2-methylpr (2×C-(H) ₃ (C)) + (1×C-(H) ₂ (C)(B)	$(1 \times C - (H)(C)_3) +$	(2×-CH₃ co	C4H9B rr (tertiary)) +
Gas phase $\Delta_i H^\circ = C_p^\circ =$	- 269.90	270.34 292.45	0.44	76STR3	Gas phase	ture – Calculated =	= Residual	Reference
Liquid pha		247.56	256	7/CTD?	$\Delta_t H^{\circ} = C_{\rho}^{\circ} =$	-111.99 109.36		
$\Delta_{i}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{i}S^{\circ} = \Delta_{i}G^{\circ} =$	-344.70	-347.56 406.68 520.10 -1257.02 27.22	2.86	76STR3	Liquid phase $\Delta_t H^\circ = C_p^\circ = 154.39$ $S^\circ =$	- 147.00 160.34 255.71	- 5.95	48KUR

TADIE	52	Bromidee	(30) _	Continued
IAHIF	7Z.	bromides	1.371 -	Continued

	pane l) ₃ (C))+(1× corr (tertian	$C-(H)(C)_2(B)$	r))+	C ₃ H ₇ Br	1,2-Dibromo (2×C-(H	pethane I) ₂ (C)(Br))	, σ = 2		C₂H₄Bı
(ZX OII)		– Calculated :	= Residual	Reference		Literatui	re – Calculated	= Residual	Reference
					Gas phase				
Gas phase					$\Delta_{\mathbf{f}}H^{\circ} =$	-37.50	-43.56	6.06	38CON/KIS
$\Delta_{\rm f}H^{\circ} =$	-97.10	- 99.79	2.69	62ROZ/AND	$C_p^{\circ} =$	85.35	75.64	9.71	69STU/WES
$C_p^{\circ} =$	88.99	88.23	0.76	69STU/WES	S° =	329.74	340.86	- 11.12	69STU/WES
S° =	316.02	321.06	-5.04	69STU/WES	$\Delta_{\mathbf{f}}S^{\circ} =$		-83.98		
$\Delta_f S^\circ =$		-229.26			$\Delta_t G^{\circ} =$		- 18.52		
$\Delta_{\mathbf{f}}G^{\circ} = $ $\ln K_{\mathbf{f}} = $		-31.44 12.68			$lnK_f =$	<u> </u>	7.47		
					Liquid phas				
Liquid phas					$\Delta_{\rm f}H^{\circ} =$	-79.20	-85.30	6.10	68WAD
	- 127.30	- 126.89	-0.41	66WAD2	$C_p^{\circ} =$	135.98	132.00	3.98	40PIT
$C_p^{\circ} =$	132.20	132.20	0.00	1881REI	$S^{\circ} = \Delta_{f}S^{\circ} =$	223.30	226.00	-2.70	40PIT
							- 198.83		
					$\Delta_f G^\circ = \ln K_f =$		-26.02 10.50		
2-Bromobu	tone			C ₄ H ₉ Br	IIIKf =		10.50		
		C-(H) ₂ (C) ₂)	+ (1 × C-(H)($C)_2(Br)), \sigma = 9$					
	Literature	- Calculated	= Residual	Reference	1,2-Dibromopropane $(1 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)(Br)) + (1 \times C - (H)(C)_2(Br)), \sigma = 3$			3r))+	C ₃ H ₆ B ₁
Gas phase					(1 > C-(1)	1)(C)2(D1));	, 0 – 3		
$\Delta_t H^\circ =$	- 120.60	- 115.90	-4.70	68WAD		Literatur	e - Calculated	= Residual	Reference
$C_p^{\circ} =$	110.79	111.12	-0.33	69STU/WES		Littiatui	c – Calculated	- Kesiduai	Reference
$S^{\circ} =$	370.28	360.22	10.06	69STU/WES		J			
$\Delta_f S^\circ =$		-326.41			Gas phase				
$\Delta_{\mathbf{f}}G^{\circ} =$		- 18.58			$\Delta_t H^\circ =$	-71.50	- 74.79	3.29	38CON/KIS
$lnK_f =$		7.49			$C_p^{\circ} =$	102.80	100.32	2.48	69STU/WES
					S° =	376.14	376.19	-0.05	69STU/WES
					$\Delta_{\mathbf{f}}S^{\circ} =$		- 184.96		
Liquid pha	ise				$\Delta_{\mathbf{f}}G^{\circ} =$		- 19.64		
$\Delta_{\rm f}H^{\circ} =$	-155.10	-148.26	-6.84	61BJE	$lnK_f =$		7.92		
$C_p^{\circ} =$	154.40	162.62	-8.22	48KUR					
					Liquid phas	e	117.67		
2 Prome 2	-methylpropa			CUD-	$\Delta_{\mathbf{f}}H^{\circ} =$	172 90	-117.57	11.00	AOVIID
$(3 \times C - (1 \times C + C))$		<-CH₃ corr (c	uaternary))+	C₄H ₉ Br	$C_p^{\circ} =$	172.80	161.72	11.08	48KUR
	Literature	e – Calculated	= Residual	Reference		$(1)_3(C) + (1$	× C-(H) ₂ (C) ₂)	+ (1 × C-(H) ₂ (C ₄ H ₈ Br
Gas phase					(1×C-(H	I)(C) ₂ (Br)),	$\sigma = J$		
$\Delta_{\rm f}H^{\circ} =$	- 131.60	-133.20	1.60	68WAD		Literatur	e - Calculated	= Residual	Reference
$C_p^{\circ} =$	116.52	116.52	0.00	69STU/WES					
S° =	331.96	331.96	0.00	69STU/WES					
$\Delta_{\mathbf{f}}S^{\circ} =$		-354.67			Gas phase				
$\Delta_{\rm f}G^{\circ} =$		-27.45			$\Delta_{\mathbf{f}}H^{\circ} =$	-92.20	-95.42	3.22	38CON/KIS
$lnK_f =$		11.07			$C_p^{\circ} =$	127.11	123.21	3.90	69STU/WES
	·····				S° =	408.78	415.35	-6.57	69STU/WES
T					$\Delta_{\mathbf{f}}S^{\circ} =$		- 282.11		
Liquid pha $\Delta_t H^\circ =$	ase 163.40	- 163.40	0.00	51BRY/HOW	$\Delta_f G^\circ = \ln K_f =$		-11.31 4.56		
		- 102,40	U.UU	JIDA I/IIUW			4.30		
					Liquid phas	e			
							142.20	2.60	61BJE
					$\Delta m = 1$	- 146.90	- 143.30	3.60	nioir.

TABLE	52	Bromides	(30) -	Continued
IARIH	JZ.	promucs	1371 -	Continucu

1,2-Dibromoheptane $(1 \times C-(H)_3(C)) + (4 \times C-(H)_2(C)_2) + (1 \times C-(H)_2(C)(C)_2(1 \times C-(H)(C)_2(Br))$	C ₇ H ₁₄ Br ₂ (Br))+	1,4-Dibromobutane $(2 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(C)(Br))$
	Reference	Literature - Calculated = Residual Reference
Gas phase $C_p^{o} = -157.90 -157.31 -0.59$ $C_p^{o} = 191.88$	41LIS	Gas phase $\Delta_l H^\circ = -87.00 -84.82 -2.18$ 68WAD $C_p^\circ = 121.42$
Liquid phase $\Delta_p H^\circ = -212.30 -220.49 8.19$ $C_p^\circ = 283.40$	41LIS	Liquid phase $\Delta_t H^\circ = -140.10 - 136.76 - 3.34$ 72ROZ/NES $C_p^\circ = 192.84$ $S^\circ = 290.76$ $\Delta_t S^\circ = -406.69$
,3-Dibromopropane $(1 \times C - (H)_2(C)_2) + (2 \times C - (H)_2(C)(Br))$	C₃H₄Br₂	$\Delta_f G^\circ = -15.50$ $\ln K_f = 6.25$ 1,3-Dibromobutane $C_4 H_8 B$
Literature Calculated = Residual	Reference	$(1 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)(Br)) + (1 \times C - (H)(C)_2(Br))$
Gas phase $\Delta_t H^\circ = -64.19$ $C_p^\circ = 98.53$		Literature - Calculated = Residual Reference
Liquid phase $\Delta_t H^\circ = -111.03$ $C_r^\circ = 158.99$ 162.42 -3.43 $S^\circ = 258.38$ $\Delta_t S^\circ = -302.76$ $\Delta_t G^\circ = -20.76$ $\ln K_t = 8.37$	48KUR	Gas phase $\Delta_t H^\circ = -95.42$ $C_p^\circ = 123.21$ Liquid phase $\Delta_t H^\circ = -147.80 -143.30 -4.50$ 72ROZ/NES $C_p^\circ = 192.14$
2,3-Dibromobutane $(2\times C-(H)_3(C)) + (2\times C-(H)(C)_2(Br)), \sigma = 18$	C ₄ H ₈ Br ₂	1,2-Dibromo-2-methylpropane $(2 \times C - (H)_3(C)) + (2 \times -CH_3 \text{ corr (quaternary)}) + (1 \times C - (C)_3(Br)) + (1 \times C - (H)_2(C)(Br))$
Literature - Calculated = Residual	Reference	Literature – Calculated = Residual Reference
•	38CON/KIS 69STU/WES	Gas phase $\Delta_t H^\circ = -113.30 - 108.16 - 5.14$ 74SUN/WUL $C_p^\circ = 128.61$
	69STU/WES	Liquid phase $\Delta_t H^\circ = -156.60 -154.05 -2.55$ 74SUN/WUL
	36TRI	2,3-Dibromo-2-methylbutane $C_5H_{10}B_1$ (3×C-(H) ₃ (C))+(1×C-(H)(C) ₂ (Br))+(1×C-(C) ₃ (Br))+ (2×-CH ₃ corr (quaternary)), $\sigma = 27$
C _p = 191.44		Literature - Calculated = Residual Reference
		Gas phase $\Delta_t H^\circ = -138.00 -139.39 \ C_\rho^\circ = 148.57 \ 153.29 -4.72 \ 69STU/WES \ S^\circ = 412.54 \ 425.79 -13.25 \ 69STU/WES \ \Delta_t S^\circ = -407.98 \ \Delta_t G^\circ = -17.75 \ \ln K_\ell = 7.16$

TABLE 52.	Bromides	(39) —	Continued
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(3×C-(H)	₃ (C))+(1×	tane (Continus C-(H)(C) ₂ (Burnary)), $\sigma = 2$	·))+(1×C-(0	$C_5H_{10}Br_2$ $C)_3(Br)) +$	3-Bromo-1-p. (1×C _d -(H		ntinued) C _d (H)(C))+(3	$1 \times C - (H)_2(C)$	$(Br), \sigma = 1$
, , , , ,		- Calculated =		Reference		Literature	- Calculated	= Residual	Reference
Liquid phase $\Delta_t H^\circ =$		-186.32			Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ =$	12.20	10.15 118.97 227.77 191.98 67.39	2.05	49GEL/SKI
1 ,2,3-Tribro r (2×C–(H)		+(1×C-(H)(C) ₂ (Br))	C ₃ H ₅ Br ₃	$lnK_f =$		-27.18		
	Literature	e — Calculated :	= Residual	Reference	1-Bromo-1-p		< C _d -(H)(C)) +	+ (1 × C,(H)(C3H5B1
Gas phase $\Delta_t H^\circ = C_p^\circ =$		54.31 112.41				rr-(alk)(X)			Reference
Liquid phase $\Delta_t H^\circ = C_p^\circ =$	e 166.52	- 112.61 191.24	- 24.72	48KUR	Gas phase $\Delta_t H^\circ = C_\rho^\circ =$	40.80	41.00 78.57	- 0.20	73ALF/GOL
Bromoethyle (1 × C _a -(F		C _a (H)(Br)), σ	- 1	C ₂ H ₃ Br	Liquid phase $C_p^{\alpha} =$	e	140.21		
	Literatur	e – Calculated	= Residual	Reference	1-Bromo-1-p (1 × C-(H		< C _d (H)(C)) +	- (1 × C(H)(C₃H₅Br Br))
Gas phase $\Delta_t H^\circ = C_p^\circ =$	79.20 55.48	77.26 55.48	1.94 0.00	57LAC/KIA2 69STU/WES			e – Calculated		Reference
$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$	275.43	275.43 -8.01 79.65 -32.13	0.00	69STU/WES	Gas phase $\Delta_t H^\circ = C_p^\circ =$	43.90	45.00 78.57	- 1.10	73ALF/GOL
Liquid phas $C_p^{\circ} =$	se 107.50	107.50	0.00	34MEH2	Liquid phase $C_p^{\circ} =$	•	140.21		
3-Bromo-1-1 (1 × C _d -(1		C _d (H)(C))+(l × C−(H)₂(C)	(Br) , $\sigma = 1$	1-Bromoprop		< C _t -(C)) + (1)	< C₁−(Βι)), σ :	C₃H₃Br = 3
	Literatur	e – Calculated	= Residual	Reference		Literature	e – Calculated	= Residual	Reference
Gas phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S^\circ$	49.37 77.66 317.15	40.86 77.94 321.88 - 97.87 70.04	8.51 - 0.28 - 4.73	69STU/WES 69STU/WES 69STU/WES	Gas phase $C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} =$	73.64 295.81	73.64 295.81 6.62	0.00 0.00	69STU/WES 69STU/WES

Table 52. Bromides (39) - Continue	TARIE	52	Bromides	(39) -	 Continue
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Bromobenzer (1×C _B -(B		$(5 \times C_B - (H)(C_B))$	$(\alpha)_2$), $\sigma = 2$	C ₆ H ₅ Br	1,2-Dibromocyclohexane $(4 \times C-(H)_2(C)_2) + (2 \times C-(H)(C)_2(Br)) + (1 \times Cyclohexane (sub) rsc)$	C ₆ H ₁₀ Br
	Literature - Calculated = Residual Reference			Reference	Literature – Calculated = Residual	Reference
Gas phase $ \Delta_t H^\circ = \\ C_p^\circ = \\ S^\circ = \\ \Delta_t S^\circ = $	105.40 97.70 324.39	105.40 97.70 324.39 -112.59	0.00 0.00 0.00	68WAD 69STU/WES 69STU/WES	Gas phase $\Delta_t H^{\circ} = -114.80 -104.41 -10.39$ $C_{\rho}^{\circ} = 142.28$	41LIS
$\Delta_f G^\circ = \ln K_f =$		138.97 -56.06			Liquid phase $\Delta_t H^\circ = -162.80 -159.60 -3.20$ $C_p^\circ = 213.95$	41LIS
Liquid phase $ \Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = S^\circ $	60.70 154.31 219.20	60.70 154.31 219.20 -217.77 125.63 -50.68	0.00 0.00 0.00	56CHE/SKI 75MAS/SCO 75MAS/SCO	1,2-Dibromocycloheptane $(5 \times C - (H)_2(C)_2) + (2 \times C - (H)(C)_2(Br)) + (1 \times Cyclored)$ Literature – Calculated = Residual	C ₇ H ₁₂ Br oheptane rsc)
Benzyl bron		(1×C _B −(C)(C _B)	₁₂)+(1×C-(1	C_7H_7Br $H)_2(C_B)(Br))$	Gas phase $\Delta_t H^\circ = -105.60 -98.31 -7.29$ $C_p^\circ = 150.85$	41LIS
Gas phase $\Delta_t H^\circ =$	Literatur	e – Calculated =	Residual	Reference 57BEN/BUS	Liquid phase $\Delta_t H^{\circ} = -157.70 -159.77$ 2.07 $C_p^{\circ} = 238.39$	41LIS
Liquid phas $\Delta_t H^\circ =$	se 15.90	15.90	0.00	63ASH/CAR	1,2-Dibromocyclooctane $(6 \times C - (H)_2(C)_2) + (2 \times C - (H)(C)_2(Br)) + (1 \times Cycl$ Literature – Calculated = Residual	C ₈ H ₁₄ B ₁ coctane rsc) Reference
(3×C-(I	opentane (s	$2 \times C - (H)(C)_2(B)$		C ₅ H ₈ Br ₂	Gas phase $\Delta_t H^\circ = -118.70 -104.63 -14.07$ $C_p^\circ = 167.71$	41LIS
Gas phase $\Delta_l H^\circ = C_p^\circ =$	- 54.90	- 63.84 114.34	8.94	41LIS	Liquid phase $\Delta_t H^\circ = -173.30 -170.90 -2.40$ $C_p^\circ = 273.12$	41LIS
Liquid phat $\Delta_t H^{\circ} = C_p^{\circ} =$	se - 102.70	-108.22 186.42	5.52	41LIS	4-Bromobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times C_B - (Br)(C_B)_2) + (1 \times O - (H)(C_B)_2) + (1 \times C_B - (CO)(C_B)_2)$	C7H4BrO H)(CO))+
					Literature – Calculated = Residual	Reference
					Gas phase $\Delta_l H^{\circ} = -272.00 -272.21$ 0.21	87FER/PIL
					Liquid phase $\Delta_t H^\circ = -362.60$ $C_p^\circ = 222.00$	

TABLE 52. Bromides (39) - Continued

TABLE 53. Iodides (39)

TABLE 32. Bromides (39) — Cont.				TABLE 33, 100	ilues (39)	
4-Bromobenzoic acid (Continued) (4 × C _B -(H)(C _B) ₂) + (1 × C _B -(Br)(C _B) ₂) + (1 × O- (1 × CO-(O)(C _B)) + (1 × C _B -(CO)(C _B) ₂)	C ₇ H ₅ BrO ₂ -(H)(CO))+	Iodomethan (1×C-(F		odide yl iodide), σ =	· 3	СН3
Literature – Calculated = Residual	Reference	•	Literatur	e – Calculated	= Residual	Reference
		Gas phase				
Solid phase		$\Delta_t H^\circ =$	14.30	14.30	0.00	65GOL/WAL
$\Delta_t H^{\circ} = -379.60 -379.38 -0.22$	87FER/PIL	$C_p^{\circ} =$	44.14	44.14	0.00	69STU/WES
$S^{\circ} = 199.44$		S° =	254.01	254.01	0.00	69STU/WES
$\Delta_t S^{\circ} = -448.32$		$\Delta_f S^\circ =$		-5.66		
$\Delta_{\rm f}G^{\circ} = -245.71$		$\Delta_{\mathbf{f}}G^{\circ} =$		15.99		
$\ln K_{\rm f} = 99.12$		$lnK_f =$		- 6.45 		
		Liquid phas	se			
Acetyl bromide	C ₂ H ₃ BrO	$\Delta_{\rm f}H^{\circ} =$	-11.70	-11.70	0.00	61CAR/CAR
$(1 \times C - (H)_3(CO)) + (1 \times CO - (C)(Br))$		C _p =	82.76	82.76	0.00	62LOW/MOE
Literature – Calculated = Residual	Reference					
		Iodoethane				C ₂ H ₅
Gas phase		(1 × C-(F	$(1)_3(C) + (1)_3(C)$	\times C-(H) ₂ (C)(I)), $\sigma = 3$	
$\Delta_t H^{\circ} = -190.80 -190.80 0.00$	26MAT		Literatur	e – Calculated	= Residual	Reference
Liquid phase						
$\Delta_t H^\circ = -223.90 -223.10 -0.80$	49CAR/SKI	Gas phase				
		$\Delta_{\rm f}H^{\circ} =$	-7.50	-8.72	1.22	68WAD
	•	$C_{\rho}^{\circ} =$	65.94	66.67	-0.73	69STU/WES
		<i>S°</i> =	296.31	295.97	0.34	69STU/WES
		$\Delta_{\mathbf{f}}S^{\circ} =$		- 100.01		
		$\Delta_{\rm f}G^{\circ} =$		21.10		
		$lnK_f =$		-8.51		
		Liquid phas				
		$\Delta_t H^{\circ} =$	- 39.50	-43.47	3.97	65ASH/CAR
		<i>C</i> _p =	115.10	101.84	13.26	48KUR
		1-Iodopropa		× C-(H)2(C)2)	+ (1 × C=/H) _*	C_3H_7
		(277.0 (2		e – Calculated		Reference
		Gas phase	···········	271 11 11 11 11 11 11 11 11 11 11 11 11 1		
		$\Delta_i H^\circ =$	- 30.84	-29.35	-1.49	69FUR/GOL
		$C_p^{\circ} =$	89.87	89.56	0.31	69STU/WES
		S° =	336.06	335.13	0.93	69STU/WES
		$\Delta_{f}S^{\circ} =$		- 197.16	- · · · -	
		$\Delta_{\rm f}G^{\circ} =$		29.43		
		$lnK_f =$		-11.87		
		Liquid phas	se			
		$\Delta_i H^\circ =$	- 67.04	-69.20	2.16	68WAD
		$C_{P}^{\circ} =$	126.80	132.26	-5.46	1881REI
						

TABLE	53.	Iodides	(39)) —	Continued
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TABLE 53. Iodides (39)

1-Iodo-3-methylbutane $(2 \times C - (H)_3(C)) + (1 \times C - (H)_2(C)$ $(2 \times - CH_3 \text{ corr (tertiary)}) + (1 \times C)$		C₅H₁₁I C) ₃) +			×-CH ₃ corr (quaternary))+	С4Н,
Literature – Calculat	ed = Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = -77.30$ $C_p^\circ = 135.37$			Gas phase $\Delta_i H^\circ = C_p^\circ = S^\circ =$	-72.00 118.28 342.21	-72.00 118.28 342.21	0.00 0.00 0.00	62BEN/AMA2 69STU/WES 69STU/WES
Liquid phase $\Delta_t H^\circ = -125.94$ $C_p^\circ = 178.70$ 190.12	-11.42	48KUR	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f =$		-326.39 25.31 -10.21		
			Liquid phas $\Delta_t H^\circ =$	e 107.40	- 107.40	0.00	68WAD
1-Iodo-2-methylpropane $(2 \times C-(H)_3(C)) + (1 \times C-(H)(C)$ $(1 \times C-(H)_2(C)(1))$	3)+(2×-CH ₃ co	C4H9I orr (tertiary))+	1,2-Diiodoet	hane			CHI
Literature – Calculat	Literature - Calculated = Residual			I) ₂ (C)(I)),	$\sigma = 2$		C ₂ H ₄ I
Gas phase				Literatui	re – Calculated	= Residual	Reference
$\Delta_{p}H^{\circ} = -56.67$ $C_{p}^{\circ} = 112.48$			Gas phase $\Delta_t H^\circ =$	66.80	67.08	-0.28	54ABR/DAV
Liquid phase $\Delta_l H^\circ = -100.21$ $C_p^\circ = 163.32$ 159.70	3.62	48KUR	$C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$	82.30 348.53	81.88 349.80 - 38.97 78.70 - 31.75	0.42 1.27	69STU/WES 69STU/WES
2-Iodopropane $(2 \times C-(H)_3(C)) + (1 \times C-(H)(C)$ $(2 \times -CH_3 \text{ corr (tertiary)}), \sigma = 0$		C ₃ H ₉ I	Liquid phas $\Delta_t H^\circ = C_p^\circ =$	e 1.10	8.28 130.72	-7.18	54ABR/DAV
Literature - Calculat	ed = Residual	Reference					
Gas phase $\Delta H^{\circ} = -39.50 -40.30$	0,80	69FUR/GOL	1,2-Diiodop: (1 × C-(H		× C-(H) ₂ (C)(I))+(1×C-(H)($C_3H_6I_2$ $C)_2(I)), \sigma = 3$
$C_p^{\circ} = 90.08$ 90.08 $S^{\circ} = 324.47$ 324.47	0.00 0.00	69STU/WES 69STU/WES		Literatur	e – Calculated	= Residual	Reference
$\Delta_t S^\circ = -338.39$ $\Delta_t G^\circ = 60.59$ $\ln K_t = -24.44$			Gas phase $\Delta_t H^\circ = C_p^\circ =$	35.60 103.64	40.02 105.29	4.42 1.65	62BEN/AMA 69STU/WES
Liquid phase $\Delta_t H^\circ = -73.60 -74.80$	1.20	68WAD	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} = 0$	395.81	384.07 -141.01 82.06 -33.10	11.74	69STU/WES
			Liquid phas $\Delta_t H^\circ =$	e	- 18.69		

Table 53. Iodides (39) — Continu

C₂H₂I)), σ = 2	cis corr-(X)(X	hylene (Z) H)(I)) + (1 \times	(2 × Cd-(1	C)(I))+	- (1 × C-(H) ₂ (
Reference	= Residual	- Calculated =	Literature		Reference	= Residual	– Calculated :		(1×0-(11)
					 				<u> </u>
68FUR/GOL	6.68	200.72	207.40	Gas phase $\Delta_t H^\circ =$					Gas phase
001 010 002	0.00	73.64	207.10	$C_p^{\circ} =$	37CLI/KIS	-7.09	19.39	12.30	$\Delta_t H^\circ =$
		333.14		S° =	69STU/WES	-0.23	128.18	127.95	$C_p^{\circ} =$
		74.95		$\Delta_{\mathbf{f}}S^{\circ} =$	69STU/WES	2.70	423.23	425.93	S° =
		178.37		$\Delta_{\mathbf{f}}G^{\circ} =$			-238.16		$\Delta_f S^\circ =$
		- 71.96		$lnK_f =$			90.40		$\Delta_{\mathbf{f}}G^{\circ} =$
	······································						- 36.47	<u> </u>	$lnK_f =$
C ₂ H ₂ I			hylene (E)	1,2-Diiodoet					Liquid phase
C21121		2	$H(I)$, $\sigma =$	•			- 44.42		$\Delta_{\rm f}H^{\circ} =$
Reference	Residual	- Calculated =	Literature						
				-	C ₃ H ₅ I		And the state of t		3-Iodo-1-pro
COET IN CO.	2.00	204.72	207.40	Gas phase	$(1)), \sigma = 1$	\times C-(H) ₂ (C)((H)(C))+(1	$(1)_2$) + $(1 \times C_0$	$(1 \times C_{d}-(H$
68FUR/GOL	2.68	204.72 73.64	207.40	$\Delta_t H^\circ =$	Reference	– Dosidual	- Calculated	T itamatuma	
		333.14		$C_p^{\circ} = S^{\circ} =$	Reference	= Residuai	- Calculated	Literature	
		74.95		$\Delta_{\rm f}S^{\circ} =$		· .			
		182.37		$\Delta_{\mathbf{f}}G^{\circ} =$					Gas phase
		-73.57		$\ln K_{\rm f} =$	66ROD/GOL	-3.08	96.18	93.10	$\Delta_t H^\circ =$
		, , , ,			69STU/WES	1.57	81.06	82.63	$C_p^{\circ} =$
					69STU/WES	-6.44	326.35	319.91	S° =
<u></u>					·	-6.44	326.35 75.37	319.91	-
С ₃ Н ₃			ne	1-Iodopropy	·	-6.44		319.91	$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} =$
	$C_{r}-(I)), \sigma =$: C _r -(C)) + (1 ×			·	-6.44	-75.37	319.91	$\Delta_f S^{\circ} =$
		: C _t -(C)) + (1 × - Calculated =	(1)₃(C))+(1×		·	-6.44	- 75.37 118.65	319.91	$\Delta_f S^\circ = \Delta_f G^\circ =$
3			(1)₃(C))+(1×		69STU/WES		-75.37 118.65 -47.86		$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phase
3			(1)₃(C))+(1×	(1×C-(H	·	-6.44 -1.71	-75.37 118.65 -47.86		$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phase $\Delta_t H^\circ = $
Reference	- Residual	- Calculated =	()₃(C))+(1× Literature	(1×C-(H	69STU/WES		-75.37 118.65 -47.86	e	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f = $ Liquid phase
Reference 69STU/WES	Residual	Calculated =	() ₃ (C)) + (1 × Literature	$(1 \times C - (H$ Gas phase $C_p^{\circ} =$	69STU/WES		-75.37 118.65 -47.86	e	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phase $\Delta_t H^\circ = $
Reference	- Residual	74.48 302.92	()₃(C))+(1× Literature	$(1 \times C - (H + C)))))))))))))))$	69STU/WES		-75.37 118.65 -47.86	e	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phase $\Delta_t H^\circ = $
Reference 69STU/WES	Residual	Calculated =	() ₃ (C)) + (1 × Literature	$(1 \times C - (H$ Gas phase $C_p^{\circ} =$	69STU/WES 49GEL/SKI		-75.37 118.65 -47.86	55.23	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phase $\Delta_t H^\circ = C_p^\circ = $
Reference 69STU/WES	Residual	74.48 302.92	() ₃ (C)) + (1 × Literature	$(1 \times C - (H + C)))))))))))))))$	69STU/WES 49GEL/SKI C3H4I		-75.37 118.65 -47.86 56.94 118.33	55.23 55.23 Spene (Z)) ₃ (C))+(1×	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-(H)}}$
Reference 69STU/WES 69STU/WES	Residual	74.48 302.92	() ₃ (C)) + (1 × Literature 74.48 302.92	Gas phase $C_p^o = S^o = \Delta_t S^o =$	69STU/WES 49GEL/SKI C3H4I	-1.71	-75.37 118.65 -47.86 56.94 118.33	55.23	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-(H)}}$
Reference 69STU/WES	0.00 0.00	74.48 302.92	() ₃ (C)) + (1 × Literature 74.48 302.92	$(1 \times C - (H \times C))))))))))))))))))))$	69STU/WES 49GEL/SKI C3H4I	– 1.71 - (1×C₄–(H)(I	-75.37 118.65 -47.86 56.94 118.33	e 55.23 ppene (Z) ₃ (C))+(1× rr-(alk)(X))	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-(H)}}$
Reference 69STU/WES 69STU/WES	0.00 0.00 0.00	74.48 302.92 31.77	$(1)_3(C)$) + $(1 \times 1)_3(C)$ + $(1 \times$	$(1 \times C - (H \times C))))))))))))))))))))$	69STU/WES 49GEL/SKI C ₃ H ₆ I	– 1.71 - (1×C₄–(H)(I	-75.37 118.65 -47.86 56.94 118.33	e 55.23 ppene (Z) ₃ (C))+(1× rr-(alk)(X))	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_\rho^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-(H)}}$
Reference 69STU/WES 69STU/WES C ₆ H ₅ I	0.00 0.00 0.00	74.48 302.92 31.77 × C _B -(H)(C _B) ₂	$(1)_3(C) + (1 \times 1)_3(C) + (1 \times 1)_$	$(1 \times C - (H \times C))))))))))))))))))))$	69STU/WES 49GEL/SKI C ₃ H ₅ I I)) + Reference	−1.71 - (1 × C _d −(H)(l = Residual	-75.37 118.65 -47.86 56.94 118.33	55.23 Spene (Z)) ₃ (C)) + (1 × rr-(alk)(X)) Literature	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-}(\text{H})}$
Reference 69STU/WES 69STU/WES C ₆ H ₅ I	0.00 0.00 0.00	74.48 302.92 31.77 × C _B -(H)(C _B) ₂	$(1)_3(C) + (1 \times 1)_3(C) + (1 \times 1)_$	$(1 \times C - (H \times C))))))))))))))))))))$	69STU/WES 49GEL/SKI C ₃ H ₆ I	– 1.71 - (1×C₄–(H)(I	-75.37 118.65 -47.86 56.94 118.33	e 55.23 ppene (Z) ₃ (C))+(1× rr-(alk)(X))	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_\rho^\circ = \frac{1-\text{Iodo-1-pro}}{(1 \times \text{C-(H})(1 \times \text{cis co}))}$
Reference 69STU/WES 69STU/WES C ₆ H ₅ I	0.00 0.00 0.00	74.48 302.92 31.77 × C _B -(H)(C _B) ₂	$(1)_3(C) + (1 \times 1)_3(C) + (1 \times 1)_$	Gas phase $C_{\rho}^{\rho} = S^{\circ} = \Delta_{f}S^{\circ} = \frac{1}{1 \times C_{B}-(I)}$ Iodobenzene $(1 \times C_{B}-(I))$	69STU/WES 49GEL/SKI C ₃ H ₅ I I)) + Reference	−1.71 - (1 × C _d −(H)(l = Residual	-75.37 118.65 -47.86 56.94 118.33 CC _d -(H)(C))+	55.23 Spene (Z)) ₃ (C)) + (1 × rr-(alk)(X)) Literature	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-}(\text{H})}$
Reference 69STU/WES 69STU/WES C ₆ H ₅ I	0.00 0.00 0.00 0.00	74.48 302.92 31.77 × C _B -(H)(C _B) ₂	() ₃ (C)) + (1 × Literature 74.48 302.92 ()(C _B) ₂) + (5 Literature	Gas phase $C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \frac{1}{1 \times C_{B}-(1)}$ Gas phase $A_{f}H^{\circ} = C_{\rho}^{\circ} = \frac{1}{1 \times C_{B}-(1)}$	69STU/WES 49GEL/SKI C ₃ H ₅ I I)) + Reference	−1.71 - (1 × C _d −(H)(l = Residual	-75.37 118.65 -47.86 56.94 118.33 CC _d -(H)(C))+	55.23 Spene (Z)) ₃ (C)) + (1 × rr-(alk)(X)) Literature	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_\rho^\circ = \frac{1-\text{Iodo-1-pro}}{(1 \times \text{C-(H})(1 \times \text{cis co}))}$
Reference 69STU/WES 69STU/WES C6H31 Reference	Residual 0.00 0.00 0.00 0.00 0.00 0.00	74.48 302.92 31.77 × C _B -(H)(C _B) ₂ - Calculated =	74.48 302.92 (I)(C _B) ₂) + (5 Literature	Gas phase $C_{\rho}^{\circ} = S^{\circ} = \Delta_{\ell}S^{\circ} = \frac{1}{1 \times C_{B}-(1)}$ Gas phase $\Delta_{\ell}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \frac{1}{1 \times C_{B}}$	49GEL/SKI C ₃ H ₅ I I))+ Reference 73ALF/GOL	−1.71 - (1 × C _d −(H)(l = Residual	-75.37 118.65 -47.86 56.94 118.33 CC _d -(H)(C))+	pene (Z)) ₃ (C))+(1× rr-(alk)(X)) Literature 86.40	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times C_t + C_t}$ Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times C_t + C_t}$
Reference 69STU/WES 69STU/WES C6H31 Reference 70COX/PIL 69STU/WES	0.00 0.00 0.00 0.00 0.00	74.48 302.92 31.77 × C _B -(H)(C _B) ₂ - Calculated = 163.55 100.75 334.05 - 84.89	74.48 302.92 2 1)(C _R) ₂) + (5 Literature	Gas phase $C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \frac{1}{1}$ Iodobenzene $(1 \times C_{B} - (1))$ Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \frac{1}{1}$	69STU/WES 49GEL/SKI C ₃ H ₅ I I))+ Reference 73ALF/GOL C ₃ H ₅ I	-1.71 $-(1 \times C_d - (H)(I)$ = Residual -6.02	-75.37 118.65 -47.86 56.94 118.33 CC _d -(H)(C))+ Calculated 92.42 81.29	pene (Z)) ₃ (C))+(1× rr-(alk)(X)) Literature 86.40	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-}(H)}$ Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-}(H)}$
Reference 69STU/WES 69STU/WES C6H31 Reference 70COX/PIL 69STU/WES	0.00 0.00 0.00 0.00 0.00	74.48 302.92 31.77 × C _B -(H)(C _B) ₂ - Calculated = 163.55 100.75 334.05 - 84.89 188.86	74.48 302.92 2 1)(C _R) ₂) + (5 Literature	Gas phase $C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \frac{1}{1}$ Iodobenzene $(1 \times C_{B} - (1))$ Gas phase $\Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \frac{1}{1}$	69STU/WES 49GEL/SKI C ₃ H ₅ I I))+ Reference 73ALF/GOL C ₃ H ₅ I	−1.71 - (1 × C _d −(H)(l = Residual	-75.37 118.65 -47.86 56.94 118.33 CC _d -(H)(C))+ Calculated 92.42 81.29	pene (Z)) ₃ (C))+(1× rr-(alk)(X)) Literature 86.40	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-}(H)}$ Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-}(H)}$
Reference 69STU/WES 69STU/WES C6H31 Reference 70COX/PIL 69STU/WES	0.00 0.00 0.00 0.00 0.00	74.48 302.92 31.77 × C _B -(H)(C _B) ₂ - Calculated = 163.55 100.75 334.05 - 84.89	74.48 302.92 2 1)(C _R) ₂) + (5 Literature	Gas phase $C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \frac{1}{1}$ Iodobenzene $(1 \times C_{B} - (1))$ Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \frac{1}{1}$	69STU/WES 49GEL/SKI C ₃ H ₅ I I))+ Reference 73ALF/GOL C ₃ H ₅ I	-1.71 $-(1 \times C_d - (H)(I)$ $= Residual$ -6.02 $-(1 \times C_d - (H)(I)$	-75.37 118.65 -47.86 56.94 118.33 CC _d -(H)(C))+ Calculated 92.42 81.29	Spene (Z) 3(C))+(1× rr-(alk)(X)) Literature 86.40 Spene (E) (3(C))+(1×	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-}(H)}$ Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-}(H)}$
Reference 69STU/WES 69STU/WES C6H31 Reference 70COX/PIL 69STU/WES	0.00 0.00 0.00 0.00 0.00	74.48 302.92 31.77 × C _B -(H)(C _B) ₂ - Calculated = 163.55 100.75 334.05 - 84.89 188.86	() ₃ (C)) + (1 × Literature 74.48 302.92 ()(C _B) ₂) + (5 Literature 164.85 100.75 334.05	Gas phase $C_{\rho}^{\rho} = S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}S^{\circ} = 1$ Iodobenzene $(1 \times C_{B} - (I))$ Gas phase $\Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = 1$ $\Delta_{f}S^{\circ} = 1$ $\ln K_{f} = 1$	69STU/WES 49GEL/SKI C ₃ H ₅ I I)) + Reference 73ALF/GOL C ₃ H ₅ I I))	-1.71 $-(1 \times C_d - (H)(I)$ $= Residual$ -6.02 $-(1 \times C_d - (H)(I)$	-75.37 118.65 -47.86 56.94 118.33 CC _d -(H)(C)) + - Calculated 92.42 81.29	Spene (Z) 3(C))+(1× rr-(alk)(X)) Literature 86.40 Spene (E) (3(C))+(1×	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-}(H)}$ Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-}(H)}$
Reference 69STU/WES 69STU/WES C6H51 Reference 70COX/PIL 69STU/WES 69STU/WES	0.00 0.00 0.00 0.00 0.00 1.30 0.00 0.00	74.48 302.92 31.77 × C _B -(H)(C _B) ₂ - Calculated = 163.55 100.75 334.05 - 84.89 188.86 - 76.18	() ₃ (C)) + (1 × Literature 74.48 302.92 ()(C _B) ₂) + (5 Literature 164.85 100.75 334.05	Gas phase $C_{\rho}^{o} = S^{\circ} = \Delta_{f}S^{\circ} =$	69STU/WES 49GEL/SKI C ₃ H ₅ I I)) + Reference 73ALF/GOL C ₃ H ₅ I I))	-1.71 $-(1 \times C_d - (H)(I)$ $= Residual$ -6.02 $-(1 \times C_d - (H)(I)$	-75.37 118.65 -47.86 56.94 118.33 CC _d -(H)(C)) + - Calculated 92.42 81.29	Spene (Z) 3(C))+(1× rr-(alk)(X)) Literature 86.40 Spene (E) (3(C))+(1×	$\Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = \ln K_{t} = \ln K_{t} = \frac{1 - \text{Iodo-1-pro}}{(1 \times \text{C-(H (1 \times \text{cis co})})^{2} + \text{C}^{\circ}_{p}} = \frac{1 - \text{Iodo-1-pro}}{(1 \times \text{C-(H (1 \times C))})})})))})}}}}}}}$
Reference 69STU/WES 69STU/WES C6H5I Reference 70COX/PIL 69STU/WES 69STU/WES	0.00 0.00 0.00 0.00 0.00 1.30 0.00 0.00	74.48 302.92 31.77 × C _B -(H)(C _B) ₂ - Calculated = 163.55 100.75 334.05 - 84.89 188.86 - 76.18	() ₃ (C)) + (1 × Literature 74.48 302.92 e ()(C _B) ₂) + (5 Literature 164.85 100.75 334.05	Gas phase $C_{\rho}^{o} = S^{o} = \Delta_{f}S^{o} = \Delta_{f}S^{o} = 1$ Iodobenzene $(1 \times C_{B} - (I))$ Gas phase $\Delta_{t}H^{o} = C_{\rho}^{o} = S^{o} = \Delta_{t}G^{o} = 1$ $Liquid phase \Delta_{t}H^{o} = S^{o} = S$	49GEL/SKI C ₃ H ₆ I I)) + Reference 73ALF/GOL C ₃ H ₅ I I)) Reference	-1.71 $-(1 \times C_d - (H)(I)$ $= Residual$ -6.02 $-(1 \times C_d - (H)(I)$ $= Residual$	-75.37 118.65 -47.86 56.94 118.33 CC _d -(H)(C)) + - Calculated 92.42 81.29 CC _d -(H)(C)) + - Calculated	Spene (Z)) ₃ (C)) + (1 × rr-(alk)(X)) Literature 86.40 Spene (E)) ₃ (C)) + (1 × Literature	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $
Reference 69STU/WES 69STU/WES C6H3I Reference 70COX/PIL 69STU/WES 69STU/WES 56SMI 37STU	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	74.48 302.92 31.77 × C _B -(H)(C _B) ₂ - Calculated = 163.55 100.75 334.05 - 84.89 188.86 - 76.18	() ₃ (C)) + (1 × Literature 74.48 302.92 ()(C _B) ₂) + (5 Literature 164.85 100.75 334.05	Gas phase $C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = 1$ Iodobenzene $(1 \times C_{B} - (1 \times C_{B$	69STU/WES 49GEL/SKI C ₃ H ₅ I I)) + Reference 73ALF/GOL C ₃ H ₅ I I))	-1.71 $-(1 \times C_d - (H)(I)$ $= Residual$ -6.02 $-(1 \times C_d - (H)(I)$	-75.37 118.65 -47.86 56.94 118.33 CC _d -(H)(C)) + - Calculated 92.42 81.29 CC _d -(H)(C)) + - Calculated	Spene (Z) 3(C))+(1× rr-(alk)(X)) Literature 86.40 Spene (E) (3(C))+(1×	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $ Liquid phase $\Delta_t H^\circ = C_p^\circ = $ 1-Iodo-1-pro $(1 \times C - (H (1 \times C) + C))$ Gas phase $\Delta_t H^\circ = C_p^\circ = $ 1-Iodo-1-pro $(1 \times C - (H (1 \times C) + C))$ Gas phase $\Delta_t H^\circ = C_p^\circ = $
Reference 69STU/WES 69STU/WES C6H5I Reference 70COX/PIL 69STU/WES 69STU/WES	0.00 0.00 0.00 0.00 0.00 1.30 0.00 0.00	74.48 302.92 31.77 × C _B -(H)(C _B) ₂ - Calculated = 163.55 100.75 334.05 - 84.89 188.86 - 76.18	() ₃ (C)) + (1 × Literature 74.48 302.92 e ()(C _B) ₂) + (5 Literature 164.85 100.75 334.05	Gas phase $C_{\rho}^{\circ} = S^{\circ} = \Delta_{f}S^{\circ} = \frac{1}{1}$ Iodobenzene $(1 \times C_{B} - (1))$ Gas phase $\Delta_{f}H^{\circ} = C_{\rho}^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \frac{1}{1}$ Liquid phase $\Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = \frac{1}{1}$ $\Delta_{f}H^{\circ} = C_{\rho}^{\circ} = S^{\circ} = S^{\circ} = \frac{1}{1}$	49GEL/SKI C ₃ H ₆ I I)) + Reference 73ALF/GOL C ₃ H ₅ I I)) Reference	-1.71 $-(1 \times C_d - (H)(I)$ $= Residual$ -6.02 $-(1 \times C_d - (H)(I)$ $= Residual$	-75.37 118.65 -47.86 56.94 118.33 CC _d -(H)(C)) + - Calculated 92.42 81.29 CC _d -(H)(C)) + - Calculated	Spene (Z)) ₃ (C)) + (1 × rr-(alk)(X)) Literature 86.40 Spene (E)) ₃ (C)) + (1 × Literature	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-(H)}}$ Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{1-\text{Iodo-1-pro}}{1 \times \text{C-(H)}}$ Gas phase
Reference 69STU/WES 69STU/WES C6H3I Reference 70COX/PIL 69STU/WES 69STU/WES 56SMI 37STU	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	74.48 302.92 31.77 × C _B -(H)(C _B) ₂ - Calculated = 163.55 100.75 334.05 - 84.89 188.86 - 76.18	() ₃ (C)) + (1 × Literature 74.48 302.92 ()(C _B) ₂) + (5 Literature 164.85 100.75 334.05	Gas phase $C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = 1$ Iodobenzene $(1 \times C_{B} - (1 \times C_{B$	49GEL/SKI C ₃ H ₆ I I)) + Reference 73ALF/GOL C ₃ H ₅ I I)) Reference	-1.71 $-(1 \times C_d - (H)(I)$ $= Residual$ -6.02 $-(1 \times C_d - (H)(I)$ $= Residual$	-75.37 118.65 -47.86 56.94 118.33 CC _d -(H)(C)) + - Calculated 92.42 81.29 CC _d -(H)(C)) + - Calculated	Spene (Z)) ₃ (C)) + (1 × rr-(alk)(X)) Literature 86.40 Spene (E)) ₃ (C)) + (1 × Literature	$\Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = \frac{1 - \text{Iodo-1-pro}}{1 - \text{Iodo-1-pro}}$ Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{1 - \text{Iodo-1-pro}}{1 \times C_p^\circ = 1 - \text{Iodo-1-pro}}$ Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{1 - \text{Iodo-1-pro}}{1 \times C_p^\circ = 1 - \text{Iodo-1-pro}}$ Gas phase $\Delta_t H^\circ = C_p^\circ = \frac{1 - \text{Iodo-1-pro}}{1 \times C_p^\circ = 1 - \text{Iodo-1-pro}}$

Benzyl iodide (5×C _B -(H	: ()(C _B) ₂)+(1	$\times C_B - (C)(C_B)$) ₂) + (1 × C-(I	C_7H_7I $H)_2(C_B)(I))$		$(C_B)_2$) + (4	e (Continued) $4 \times C_B - (H)(C_B)$	$)_2) + (1 \times C_B - ($	C_7H_7I $C)(C_B)_2) +$
	Literature	- Calculated	= Residual	Reference		Literatur	e – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ =$	100.00	100.00	0.00	57BEN/BUS	Liquid phase $\Delta_t II^\circ = C_p^\circ =$	67.50	77.89 182.47	- 10.39	56SMI
Liquid phase $\Delta_t H^\circ =$	52.72	52.72	0.00	63ASH/CAR	$S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = 0$		240.36 -314.89 171.77 -69.29		
	$(C_B)_2) + (4$	×C _B -(H)(C _B)		C_7H_7I $C)(C_B)_2) +$					
	Literature	e – Calculated	= Residual	Reference	1-Iodonaphtl (1×C _B -(I)		$7 \times C_B - (H)(C_B)$	$(2 \times C_{BF})$	$(C_{BF})(C_B)_2$
Gas phase			0.00	gogov my		Literatur	e – Calculated	= Residual	Reference
$\Delta_t H^\circ = C_p^\circ =$	132.80	133.63 122.62	-0.83	70COX/PIL	Gas phase $\Delta_t H^\circ - C_p^\circ =$	233.90	231.37 127.97	2.53	70COX/PIL
Liquid phase $ \Delta_t H^\circ = C_t^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = $	78.40	84.19 182.47 240.36 -314.89 178.07 -71.83	-5.79	56SMI	Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = S^\circ = S$	161.50	162.48 222.97 252.09 - 320.38 258.00	- 0.98	56SMI
1-Iodo-3-me (1 × C _B -(1 (1 × C-(H	$((C_B)_2) + (4)_3(C)$	e l×C _B -(H)(C _B) e – Calculated		C_7H_7 $C)(C_B)_2) +$ Reference	$ \frac{\ln K_{\rm f}}{=} $ Solid phase $ \Delta_{\rm f} H^{\circ} = C_{\rm p}^{\circ} = $		- 104.08 144.31 185.59		
Gas phase $\Delta_t H^\circ = C_p^\circ =$	133.60	131.12 122.62	2.48	70COX/PIL	2-Iodonaphti (1×C _B -(I)		7×С _в -(H)(Св))2) + (2 × C _{BF}	C ₁₆ H ₇ l (C _{BF})(C _B) ₂)
Liquid phas	е					Literatur	e – Calculated	= Residual	Reference
$\Delta_{t}H^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}G^{\circ} = \ln K_{t} = 0$	79.20	77.89 182.47 240.36 -314.89 171.77 -69.29	1.31	56SMI	Gas phase $\Delta_t H^\circ = C_p^\circ =$	235.15	231.37 127.97	3.78	70COX/PIL
1-Iodo-4-me	$I(C_B)_2 + (4_{13}(C))$			C_7H_7I $C)(C_B)_2) +$ Reference	Liquid phase $\Delta_t H^\circ = C_b^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t = 0$		162.48 222.97 252.09 - 320.38 258.00 - 104.08		
Gas phase $\Delta_t H^\circ = C_p^\circ =$	121.90	131.12 122.62	-9.22	70COX/PIL	Solid phase $\Delta_t H^\circ = C_p^\circ =$	144.35	144.31 185.59	0.04	56SMI

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TABLE 53. Iodides (39) - Continued

	enzene H)(C_B) ₂) + (corr-(I)(I))	$(2 \times C_B - (I)(C_B))$ $\sigma = 2$	2)+	C ₆ H ₄ I ₂	1,4-Diiodobe $(4 \times C_B - (1 \times C_B))$	$I)(C_B)_2) +$	(2×C _B -(I)(C _B		C ₆ H ₄ I ₂
	Literatur	e – Calculated =	= Residual	Reference		Literatur	c Calculated	- Residual	Reference
Gas phase $\Delta_t H^\circ = C_p^\circ =$	251.88	251.80 119.84	0.08	70COX/PIL	Gas phase $\Delta_t H^\circ = C_p^\circ =$	· · · · · · · · · · · · · · · · · · ·	244.24 119.84		
$S^{\circ} = \Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} = \ln K_{f} =$		384.00 - 27.73 260.07 - 104.91			Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ =$	•	180.04 181.06 237.64		
Liquid phas $\Delta_t H^\circ = C_p^\circ =$	se 187.00	187.00 181.06	0.00	56SMI2	$\Delta_f S^\circ = \Delta_f G^\circ = \ln K_f = -1$	······································	-174.08 231.94 -93.56		
$S^{\circ} = \Delta_f S^{\circ} = \Delta_f G^{\circ} = \ln K_f =$		237.64 - 174.08 238.90 - 96.37			Solid phase $\Delta_t H^\circ = C_p^\circ =$	160.70	166.92 160.68	-6.22	56SMI
Solid phase $\Delta_l H^\circ = C_p^\circ =$	172.40	172.42 160.68	-0.02	56SMI	Iodocyclohex (5×C-(H (1×Cyclo		I × C-(H)(C) ₂ (I b) rsc)	I))+	C₅H₁₁I
					` '	•	, ,		
1,3-Diiodob		(0×0 (1)(C)	\ . /1 \	C ₆ H ₄ I ₂		Literatur	e – Calculated	= Residual	Reference
•	$(H)(C_B)_2) +$	(2×C _B -(I)(C _B)			Gas phase $\Delta_t H^\circ = C_p^\circ =$	Literatur	e – Calculated – 54.80 130.25	= Residual	Reference 56BRE/UBB
•	$(H)(C_B)_2) +$			corr-(I)(I))	$\Delta_t H^\circ = C_p^\circ =$ Liquid phase	-50.00	-54.80	· · · · · · · · · · · · · · · · · · ·	
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phat $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$	(H)(C _B) ₂) + Literatur	244.24 119.84 180.04 181.06		corr-(I)(I))	$\Delta_l H^\circ = C_p^\circ = $ Liquid phase $\Delta_l H^\circ = $ 1,3-Diiodocy	50.00 97.20	- 54.80 130.25 - 105.93	4.80	56BRE/UBB 56SMI C4H6I2
Gas phase $\Delta_t H^\circ = C_p^\circ = $ Liquid phase $\Delta_t H^\circ = C_p^\circ $	(H)(C _B) ₂) + Literatur	244.24 119.84		corr-(I)(I))	$\Delta_l H^\circ = C_p^\circ = $ Liquid phase $\Delta_l H^\circ = $ 1,3-Diiodocy	-50.00 -97.20 clobutane(a)2(C)2) + (2	- 54.80 130.25 - 105.93	4.80 8.73	56BRE/UBB 56SMI C ₄ H ₆ I ₂
Gas phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phat $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $C_{p}^{\circ} = \Delta_{t}S^{\circ} =$ $\Delta_{t}G^{\circ} =$	(H)(C _B) ₂) + Literatur	244.24 119.84 180.04 181.06 237.64 -174.08 231.94		corr-(I)(I))	$\Delta_l H^\circ = C_p^\circ = $ Liquid phase $\Delta_l H^\circ = $ 1,3-Diiodocy	-50.00 -97.20 clobutane(a)2(C)2) + (2	-54.80 130.25 -105.93 cis/trans)	4.80 8.73	56SMI C ₄ H ₆ I ₂ butane rsc)

2-Iodophenol $(4 \times C_{B}-(H))$ $(1 \times O-(H))$	$I(C_B)_2 + (1$	$\times C_B - (I)(C_B)_2$	$(1 \times C_B - (1 \times C_B))$	C_6H_5IO $O)(C_B)_2) +$	4-Iodophenol (Contin $(4 \times C_B-(H)(C_B)_2)$ - $(1 \times O-(H)(C_B))$		₂) + (1 × C _B -(C ₆ H ₅ IO O)(C _B) ₂) +
	Literature	– Calculated =	= Residual	Reference	Literati	ure – Calculated =	Residual	Reference
Gas phase					Liquid phase			
$\Delta_t H^{\circ} =$		- 15.31			$\Delta_t H^\circ =$	-91.02		
$C_{\rho}^{\circ} =$		121.16			$C_p^{\circ} =$	220.24		
					S° =	209.86		
					$\Delta_{\rm f} S^{\circ} :=$	-311.60		
Liquid phase	e				$\Delta_{\rm f}G^{\circ} =$	1.88		
$\Delta_t H^\circ =$		-91.02			$lnK_f =$	-0.76		
$C_p^{\circ} =$		220.24						
S° =		209.86						
$\Delta_f S^\circ =$		-311.60			Solid phase			
$\Delta_t G^\circ =$		1.88			$\Delta_t H^{\circ} = -95.40$	- 101.73	6.33	56SMI
$lnK_f =$		-0.76			$C_p^{\circ} =$	149.56		
Solid phase								
$\Delta_t H^\circ = C_p^\circ =$	-95.80	-101.73 149.56	5.93	56SMI	3-Iodopropanoic acid $(1 \times O-(H)(CO)) +$ $(1 \times C-(H)_2(C)(I))$		+ (1 × C-(H)	C3H5IO2)2(CO)(C)) +
					Literati	ure ~ Calculated =	Residual	Reference
3-Iodopheno	oli			C4H4IO				
		$1 \times C_B - (I)(C_B)$	$_2) + (1 \times C_{B} - ($	O)(C _B) ₂) !				
(1×O-(H			2) (/(-/-/	Gas phase $\Delta_t H^\circ =$	270.94		
	Literature	- Calculated =	= Residual	Reference	$C_{\rho}^{\circ} =$	- 379.84 106.42		
·		<u>,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,</u>						
Gas phase					Liquid phase			
Gas phase $\Delta_t H^\circ =$		- 15.31			Liquid phase $\Delta_t H^\circ =$	- 455.01		
Gas phase $\Delta_t H^\circ = C_p^\circ =$		-15.31 121.16				- 455.01 177.45		
$\Delta_t H^\circ = C_p^\circ = -$					$\Delta_i H^\circ = C_p^\circ =$			· · · · · · · · · · · · · · · · · · ·
$\Delta_t H^\circ = C_p^\circ = $ Liquid phas	e	121.16			$\Delta_t H^\circ = C_p^\circ = $ Solid phase	177.45	0.00	44POT
$\Delta_t H^\circ = C_p^\circ = $ Liquid phas $\Delta_t H^\circ = $		121.16 -91.02	- 4 - 14 - 17 - 17 - 1 7		$\Delta_i H^\circ = C_p^\circ =$		0.00	44ROT
$\Delta_t H^\circ = C_p^\circ = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = $	e	121.16 - 91.02 220.24			$\Delta_t H^\circ = C_p^\circ = $ Solid phase	177.45	0.00	44ROT
$\Delta_t H^\circ = C_p^\circ = $ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = $	e ·	- 91.02 220.24 209.86			$\Delta_t H^\circ = C_p^\circ = $ Solid phase	177.45	0.00	44ROT
$\Delta_t H^\circ = C_p^\circ = C_p^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = S^$	e	-91.02 220.24 209.86 -311.60			$\Delta_t H^\circ = C_p^\circ =$ $C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$	177.45	0.00	
$\Delta_t H^\circ = C_p^\circ = C_p^\circ = C_p^\circ = C_p^\circ = S_p^\circ = \Delta_t S_p^\circ = \Delta_t G_p^\circ = C_p^\circ = C_$	æ	-91.02 220.24 209.86 -311.60 1.88			$\Delta_t H^\circ = C_\rho^\circ = $ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid	177.45 - 460.00		C7HsIO2
$\Delta_t H^\circ = C_p^\circ = C_p^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = S^$	e	-91.02 220.24 209.86 -311.60			$\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (4.5)$	177.45 - 460.00 + (1×C _B -(I)(C _B) ₂)+(1×O-(F	C7HsIO2
$\Delta_t H^\circ = C_p^\circ = C_p^\circ = C_p^\circ = C_p^\circ = S_p^\circ = \Delta_t S_p^\circ = \Delta_t G_p^\circ = C_p^\circ = C_$	e	-91.02 220.24 209.86 -311.60 1.88		· · · · · · · · · · · · · · · · · · ·	$\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + (1 \times CO - (O$	177.45 -460.00 +(1×C _B -(I)(C _B) ₂ +(1×C _B -(CO)(C)+(1×O-(F	C7HsIO2
$\Delta_t H^{\circ} = C_p^{\circ} =$ Liquid phas $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \Delta_t G^{\circ} = \ln K_t =$	e	-91.02 220.24 209.86 -311.60 1.88		· · · · · · · · · · · · · · · · · · ·	$\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (4.5)$	177.45 -460.00 +(1×C _B -(I)(C _B) ₂ +(1×C _B -(CO)(C)+(1×O-(F	C7HsIO2
$\Delta_t H^\circ = C_p^\circ =$ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t =$ Solid phase		-91.02 220.24 209.86 -311.60 1.88 -0.76	7.12	54CMI	$\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + (1 \times ortho \text{ corr-}(I)(C_B)_2) + (1 \times ortho \text{ corr-}(I$	177.45 -460.00 + (1×C _B -(I)(C _B) ₂ + (1×C _B -(CO)(CCOOH))) + (1 × O–(F B)2) +	C ₇ H ₅ IO ₂ H)(CO)) +
$\Delta_t H^\circ = C_p^\circ =$ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$	- 94.50	-91.02 220.24 209.86 -311.60 1.88	7.23	56SMI	$\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + (1 \times ortho \text{ corr-}(I)(C_B)_2) + (1 \times ortho \text{ corr-}(I$	177.45 -460.00 +(1×C _B -(I)(C _B) ₂ +(1×C _B -(CO)(C) + (1 × O–(F B)2) +	C7HsIO2
$\Delta_t H^{\circ} = C_p^{\circ} =$ Liquid phas $\Delta_t H^{\circ} = C_p^{\circ} = S^{\circ} = \Delta_t S^{\circ} = \ln K_t =$ Solid phase $\Delta_t H^{\circ} = \infty$		-91.02 220.24 209.86 -311.60 1.88 -0.76	7.23	56SMI	$\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) - (1 \times CO - (O)(C_B)) + (1 \times ortho \text{ corr-}(I)(C_B)_2)$ Literatu	177.45 -460.00 + (1×C _B -(I)(C _B) ₂ + (1×C _B -(CO)(CCOOH))) + (1 × O–(F B)2) +	C ₇ H ₅ IO ₂ H)(CO)) +
$\Delta_t H^\circ = C_p^\circ =$ Liquid phas $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \ln K_t =$ Solid phase $\Delta_t H^\circ =$		-91.02 220.24 209.86 -311.60 1.88 -0.76	7.23	56SMI	Solid phase $\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) - (1 \times CO - (O)(C_B)) - (1 \times ortho \text{ corr-}(I)(C_B))$ Literatu	177.45 -460.00 +(1×C _B -(I)(C _B) ₂ +(1×C _B -(CO)(CCOOH))) + (1 × O–(F B)2) +	C ₇ H ₅ IO ₂ H)(CO)) +
$\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = \Delta_t G^\circ = \ln K_t =$ Solid phase $\Delta_t H^\circ = C_p^\circ = \Delta_t H^\circ = C_p^\circ = \Delta_t H^\circ = \Delta_t H^\circ$	– 94.50 ol	-91.02 220.24 209.86 -311.60 1.88 -0.76	· · · · · · · · · · · · · · · · · · ·	C¢H₃IO	$\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) - (1 \times CO - (O)(C_B)) + (1 \times ortho \text{ corr-}(I)(C_B)_2)$ Literatu	177.45 -460.00 +(1×C _B -(I)(C _B) ₂ +(1×C _B -(CO)(COOH)) ure - Calculated =) + (1 × O–(F B)2) +	C ₇ H ₅ IO ₂ H)(CO)) +
$\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = 1$ $\Delta_t G^\circ = 1$ $\Delta_t H^\circ = C_p^\circ = 1$ Solid phase $\Delta_t H^\circ = C_p^\circ = 1$	– 94.50 ol	-91.02 220.24 209.86 -311.60 1.88 -0.76	· · · · · · · · · · · · · · · · · · ·	C¢H4IO	$\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) - (1 \times CO - (O)(C_B)) + (1 \times ortho \text{ corr-}(I)(C_B)_2)$ Literatu	177.45 -460.00 +(1×C _B -(I)(C _B) ₂ +(1×C _B -(CO)(COOH)) ure - Calculated =) + (1 × O–(F B)2) +	C ₇ H ₅ IO ₂ H)(CO)) +
$\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phase $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $S^{\circ} = \Delta_{t}S^{\circ} =$ $\Delta_{t}G^{\circ} =$ $\ln K_{f} =$ Solid phase $\Delta_{t}H^{\circ} =$ $C_{p}^{\circ} =$	– 94.50 ol H)(С _в) ₂) + (-91.02 220.24 209.86 -311.60 1.88 -0.76	· · · · · · · · · · · · · · · · · · ·	C¢H4IO	$\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + (1 \times ortho \text{ corr-}(I)(C_B)_2) + (1 \times ortho \text{ corr-}$	177.45 -460.00 +(1×C _B -(I)(C _B) ₂ +(1×C _B -(CO)(COOH)) ure - Calculated =) + (1 × O–(F B)2) +	C ₇ H ₅ IO ₂ H)(CO)) +
$\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = 10 \text{ m/s}^\circ = 10 \text{ m/s}^$	– 94.50 ol H)(С _в) ₂) + (-91.02 220.24 209.86 -311.60 1.88 -0.76	· · · · · · · · · · · · · · · · · · ·	C¢H4IO	$\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + (1 \times ortho \text{ corr-}(I)(C_B)_2) + (1 \times ortho \text{ corr-}$	177.45 -460.00 +(1×C _B -(I)(C _B) ₂ +(1×C _B -(CO)(COOH)) ure - Calculated =) + (1 × O–(F B)2) +	C ₇ H ₅ IO ₂ H)(CO)) +
$\Delta_t H^\circ = C_p^\circ =$ Liquid phase $\Delta_t H^\circ = C_p^\circ = S^\circ = \Delta_t S^\circ = 10 \text{ m/s}^\circ = 10 \text{ m/s}^$	- 94.50 ol H)(C _B) ₂)+(-91.02 220.24 209.86 -311.60 1.88 -0.76	₂)+(1×C _B -(C¢H4IO	$\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + (1 \times ortho \text{ corr-}(I)(C_B)_2) + (1 \times ortho \text{ corr-}$	177.45 -460.00 +(1×C _B -(I)(C _B) ₂ +(1×C _B -(CO)(CCOOH)) are - Calculated = -214.06) + (1 × O–(F B)2) +	C ₇ H ₅ IO ₂ H)(CO)) +
$\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ Liquid phas $\Delta_{t}H^{\circ} = C_{p}^{\circ} =$ $S^{\circ} = \Delta_{t}S^{\circ} =$ $\Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} =$ $\Delta_{t}H^{\circ} =$ Solid phase $\Delta_{t}H^{\circ} =$ $C_{p}^{\circ} =$ 4-lodophene $(4 \times C_{B} - (1 \times O_{T}) + (1 \times O_{T}))$	- 94.50 ol H)(C _B) ₂)+(121.16 -91.02 220.24 209.86 -311.60 1.88 -0.76 -101.73 149.56	₂)+(1×C _B -(C ₆ H ₅ IO O)(C _B) ₂)+	$\Delta_t H^\circ = C_\rho^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) - (1 \times CO - (O)(C_B)) + (1 \times ortho \text{ corr-}(I)(C_B)_2) - (1 \times ortho \text{ corr-}$	177.45 -460.00 +(1×C _B -(I)(C _B) ₂ +(1×C _B -(CO)(CCOOH)) are - Calculated = -214.06 -308.80) + (1 × O–(F B)2) +	C ₇ H ₅ IO ₂ I)(CO)) +
$\Delta_t H^\circ = C_p^\circ =$ Liquid phas $\Delta_t H^\circ = S_p^\circ = $	- 94.50 ol H)(C _B) ₂)+(121.16 -91.02 220.24 209.86 -311.60 1.88 -0.76 -101.73 149.56 1 × C _B -(I)(C _B)	₂)+(1×C _B -(C ₆ H ₅ IO O)(C _B) ₂)+	$\Delta_t H^\circ = C_p^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) - (1 \times CO - (O)(C_B)) + (1 \times ortho \text{ corr-}(I)(C_B)_2) - (1 \times ortho \text{ corr-}$	177.45 -460.00 +(1×C _B -(I)(C _B) ₂ +(1×C _B -(CO)(CCOOH)) are - Calculated = -214.06 -308.80 226.26) + (1 × O–(F B)2) + • Residual	C7H5IO2 I)(CO)) + Reference
$\Delta_{t}H^{\circ} = C_{p}^{\circ} = C_{p}^{\circ} = C_{p}^{\circ} = C_{p}^{\circ} = C_{p}^{\circ} = S^{\circ} = \Delta_{t}S^{\circ} = \Delta_{t}S^{\circ} = \ln K_{t} = C_{p}^{\circ} = \ln K_{t} = C_{p}^{\circ} = C_{p}^{\circ}$	- 94.50 ol H)(C _B) ₂)+(121.16 -91.02 220.24 209.86 -311.60 1.88 -0.76 -101.73 149.56	₂)+(1×C _B -(C ₆ H ₅ IO O)(C _B) ₂)+	$\Delta_t H^\circ = C_\rho^\circ =$ Solid phase $\Delta_t H^\circ = -460.00$ 2-Iodobenzoic acid $(4 \times C_B - (H)(C_B)_2) - (1 \times CO - (O)(C_B)) + (1 \times ortho \text{ corr-}(I)(C_B)_2) - (1 \times ortho \text{ corr-}$	177.45 -460.00 +(1×C _B -(I)(C _B) ₂ +(1×C _B -(CO)(CCOOH)) are - Calculated = -214.06 -308.80) + (1 × O–(F B)2) +	C ₇ H ₅ IO ₂ H)(CO)) +

TABLE 53. Iodides (39) — Continued	TARIF	53	Indides	(39) -	Continued
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	$(1 \times C_B - (I)(C_B) + (1 \times C_B - (I)(C_B)) + (1 \times C_B - (CO)(C_B))$		C ₇ H ₅ IO ₂ H)(CO)) +	Methyl 3-iodobenzoad $(4 \times C_B - (H)(C_B)_2) - (1 \times CO - (O)(C_B))$	$+(1\times C_B-(I)(C_B)$		
Liter	ature – Calculated	= Residual	Reference	Literati	ure – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ =$	-214.06			Gas phase $\Delta_t H^\circ =$	- 190.89		
Liquid phase $\Delta_t H^\circ = C_p^\circ =$	- 308.80 226.26			Liquid phase $\Delta_t H^\circ = C_p^\circ =$	- 266.79 244.50		
Solid phase $\Delta_t H^{\circ} = -316.9$ $C_p^{\circ} =$	00 -322.48 166.06	5.58	56SMI	Solid phase $\Delta_t H^\circ = -278.30$ $C_p^\circ =$	- 297.67 182.91	19.37	56SMI
$(1 \times CO - (O)(C_B)$	$(1 \times C_{B} - (1)(C_{B}) + (1 \times C_{B} - (1)(C_{B})) + (1 \times C_{B} - (CO)(1))$	$(C_B)_2$		Methyl 4-iodobenzoat $(4 \times C_B - (H)(C_B)_2) + (1 \times CO - (O)(C_B)) + (1 \times CO - (O)(C_B$	$+(1\times C_B-(I)(C_B)$ $+(1\times O-(C)(CO)$))+(1×C-(H	I)₃(O))
Lite	rature – Calculated	= Residual	Reference	Literati	ure – Calculated	= Residual	Reference
Gas phase $\Delta_t H^\circ = -228.2$	20 –214.06	- 14.14	70COX/PIL	Gas phase $\Delta_t H^\circ =$	- 190.89		
Liquid phase $\Delta_t H^\circ = C_p^\circ =$	-308.80 226.26			Liquid phase $\Delta_t H^\circ = C_p^\circ =$	- 266.79 244.50		
Solid phase $\Delta_t H^{\circ} = -316.5$ $C_p^{\circ} =$	10 -322.48 166.06	6.38	56SMI	Solid phase $\Delta_t H^\circ = -286.60$ $C_p^\circ =$	297.67 182.91	11.07	56SMI
Methyl 2-iodobenz (4×C _B -(H)(C _B) (1×CO-(O)(C _E	coate $(1) + (1 \times C_B - (1)(C_B + (1) \times C_B - (1)(C_B + (1)(C_$	() ₂) + (1 × C _B -(())) + (1 × C-(F	C ₈ H ₇ IO ₂ CO)(C _B) ₂) + I) ₃ (O))	Acetyl iodide (1×C-(H) ₃ (CO))+	· (1 × CO-(C)(I))		C₂H₃IO Reference
Lite	rature – Calculated	= Residual	Reference			- 1000000	
Gas phase $\Delta_t H^\circ =$	- 190.89			Gas phase $\Delta_l H^{\circ} = -126.20$	- 126.20	0.00	70COX/PIL
				Liquid phase			

TABLE 54.	Mixed	Halogen	Compounds	(18))
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TABLE 54. Mixed Halogen Compounds (18) - Continued

1-Chloro-1-fluoroethane $(1 \times C - (H)_3(C)) + (1 \times C - (H)(C)(Cl)(F))$	C ₂ H ₄ CIF	1-Chloro-1,1,3,3,3-pentafluoropropane $(1\times C-(C)(Cl)(F)_2) + (1\times C-(H)_2(C)_2) + (1\times C-(G)_2(C)_2) + (1\times C-(G)_2(C)_2(C)_2) + (1\times C-(G)_2(C)_2(C)_2(C)_2(C)_2(C)_2(C)_2(C)_2(C$	C ₃ H ₂ CIF ₅ (C)(F) ₃) Reference	
Literature - Calculated = Residual	Reference	Literature – Calculated = Residual		
Gas phase $\Delta_t H^{\circ} = -313.40 - 313.40 = 0.00$ 1,1,1-Trifluoro-2-iodoethane	73KOL/PAP C ₂ H ₂ F ₃ I	Liquid phase $\Delta_t H^\circ = -1180.90 - 1200.80 \qquad 19.90$ $C_P^\circ = 196.48 \qquad 187.24 \qquad 9.24$ $S^\circ = 311.62 \qquad 306.25 \qquad 5.37$ $\Delta_t S^\circ = \qquad -459.73$ $\Delta_t G^\circ = \qquad -1063.73$ $\ln K_f = \qquad 429.10$	73SLA/KOL 74VOR/KOL 74VOR/KOL	
$(1 \times C - (C)(F)_3) + (1 \times C - (H)_2(C)(I))$		$\ln K_{\rm f} = 429.10$		
Literature – Calculated = Residual	Reference	1270	a= =	
Gas phase $\Delta_t H^\circ = -644.50 -640.27 -4.23$ $C_p^\circ = 93.93$	74WU/ROD	1,2-Dibromotetrafluoroethane (2×C-(C)(Br)(F) ₂) Literature – Calculated = Residual	C ₂ Br ₂ F.	
1,2-Dibromo-1,2-dichloroethane (2×C-(H)(C)(Br)(Cl))	C ₂ H ₂ Br ₂ Cl ₂	Gas phase $\Delta_t H^\circ = -789.10 -789.10$ 0.00	56LAC/CAS	
Literature - Calculated = Residual Gas phase	Reference	Liquid phase $C_{\rho}^{\circ} = 170.79 170.80 -0.01$ $S^{\circ} - 299.41 299.40 0.01$ $\Delta_{\rho}S^{\circ} = -269.65$	82KOS/ZHO 82KOS/ZHO	
$C_p^{\text{Hos}} = -36.90 - 36.90 0.00$ $C_p^{\text{o}} = 103.76$	39MUL/SCH	12 Phillipset of Ground	9.01.7	
3,3-Dichloro-1,1,1-trifluoropropane $(1\times C-(C)(F)_3)+(1\times C-(II)_2(C)_2)+(1\times C-(II)_3(C)_3)$	C ₃ H ₃ Cl ₂ F ₃	1,2-Dichlorotetrafluoroethane (2×C-(C)(Cl)(F) ₂) Literature – Calculated – Residual	C ₂ Cl ₂ F.	
Literature – Calculated = Residual	Reference	Gas phase		
Gas phase $\Delta_t H^\circ = -803.50 -773.54 -29.96$	72KOL/SLA3	$\Delta_t H^\circ = -925.40 -925.40$ 0.00 $C_p^\circ = 114.64$	82PAP/KOL	
$C_p^{\circ} =$ 126.57 Liquid phase $\Delta_t H^{\circ} = -837.40 -837.40 0.00$ $C_p^{\circ} = 191.29 188.62 2.67$ $S^{\circ} = 295.06 296.39 -1.33$ $\Delta_t S^{\circ} = -443.68$ $\Delta_t G^{\circ} = -705.12$ $\ln K_t = 284.44$	72KOL/SLA3 72KOL/VOR 72KOL/VOR	Liquid phase $\Delta_t H^\circ = -939.70 -932.00 -7.70$ $C_p^\circ = 164.01 167.28 -3.27$ $S^\circ = 282.00 276.62 5.38$ $\Delta_t S^\circ = -363.20$ $\Delta_t G^\circ = -823.71$ $\ln K_f = 332.28$	37PER 81KOL/KOS 81KOL/KOS	
I-Chloro-1,1,3,3,3-pentafluoropropane	C ₃ H ₂ ClF ₅	1,1,2-Trichloro-1,2,2-trifluoroethane $(1\times C-(C)(Cl)_2(F))+(1\times C-(C)(Cl)(F)_2)$	C ₂ Cl ₃ F ₃	
$(1 \times C - (C)(C1)(F)_2) + (1 \times C - (H)_2(C)_2) + (1 \times C - (H)_2(C)_$		Literature – Calculated = Residual	Reference	
Literature – Calculated = Residual	Reference	Gas phase $\Delta_t H^\circ = -777.30 -785.24$ 7.94	68KOL/TAL	
Gas phase $\Delta_t H^\circ = -1154.00 -1157.14$ 3.14 $C_\rho^\circ = 133.20$	73SLA/KOL	1,1,00 100,07 1,27		

TABLE 54. Mixed halogen comp	oounds (18) -	- Continued	TABL	E 54. Mixe	d halogen com	pounds (18)	- Continued
1,1,2-Trichloro-1,2,2-trifluoroethane ($(1 \times C - (C)(C))_2(F)$) + $(1 \times C - (C)(C)$		C ₂ Cl ₃ F ₃			ne (Continued) + (1 × C-(H) ₂ (C		C₂H₄Br(
Literature – Calculated =	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Liquid phase			Liquid phas	se			
$\Delta_t H^\circ = -805.80 -809.87$	4.07	63HIR/HIL	$\Delta_{\rm f}H^{\circ} =$		- 129.55		
$C_p^{\circ} = 172.80 172.93$	-0.13	81KOL/KOS	$C_{\rho}^{\circ} =$	130.12	129.76	0.36	39RAI
$S^{\circ} = 289.53 280.02$	9.51	81KOL/KOS	S° =		217.27		
$\Delta_{\rm f} S^{\circ} = -369.94$			$\Delta_f S^\circ =$		- 242.94		
$\Delta_{\rm f}G^{\circ} = -699.57$			$\Delta_{\rm f}G^{\circ} =$		-57.12		
$\ln K_{\rm f} = 282.20$			$lnK_f =$		23.04		
1-Chloro-1,1-difluoroethane		C ₂ H ₃ ClF ₂	1 1 1 Trich	laro-3 3 3-tr	ifluoropropane		C₃H₂Cl₃F
$(1 \times C - (H)_3(C)) + (1 \times C - (C)(Cl)(F)$)2)	C2113C112			$1 \times C - (C)(Cl)_3$		
Literature Calculated	= Residual	Reference		Literatu	re – Calculated	= Residual	Reference
Gas phase			Gas phase				
$\Delta_{\rm f}H^{\circ} = -504.96$			$\Delta_{\rm f}H^{\circ} =$		<i>−776.42</i>		
$C_p^{\circ} = 83.05$			$C_{\rho}^{\circ} =$		144.06		
Liquid phase			Liquid phas	se			
$\Delta_t H^{\circ} = -513.61$			$\Delta_{\rm f}H^{\circ} =$		847.73		
$C_p^{\circ} = 131.40$ 120.12 $S^{\circ} = 221.61$	11.28	42REI	$C_p^{\circ} =$	199.91	205.80	-5.89	71KOL/VOR
$S^{\circ} = 221.61$ $\Delta_f S^{\circ} = -299.89$			S° =	311.42	313.85	-2.43	71KOL/VOR
$\Delta_{f}G^{\circ} = -299.89$ $\Delta_{f}G^{\circ} = -424.20$			$\Delta_{f}S^{\circ} = \Delta_{f}G^{\circ} =$		- 472.42 - 706.88		
$\ln K_{\rm f} = 171.12$			$\ln K_{\rm f} =$		285.15		
1,2-Diffuorotetrachloroethane (2×C-(C)(Cl) ₂ (F))		C ₂ Cl ₄ F ₂	1-Chloro-3, (1×C-(F		opropane ' + (1 × C-(H) ₂ (C) ₂) + (1 × C-(C3H4CIF3 (C)(F)3)
Literature - Calculated	= Residual	Reference			e – Calculated		Reference
Gas phase			Gas phase				
$\Delta_t H^\circ = -645.08$			$\Delta_{\rm f} H^{\circ} =$		- 763.89		
			$C_p^{\circ} =$		113.41		
Liquid phase $\Delta_t H^\circ = -687.74$			Liquid phas	se			
$C_p^{\circ} = 178.57$ 178.58	-0.01	78KIS/SUG	$\Delta_t H^{\circ} =$		-821.70		
$S^{\circ} = 283.42 283.42$	0.00	78KIS/SUG	C_p° -	171.08	167.36	3.72	74KOL/VOR
$\Delta_t S^\circ = -376.69$			S° =	271.67	272.21	-0.54	74KOL/VOR
$\Delta_t G^{\circ} = -575.43$			$\Delta_{\rm f}S^{\circ} =$		-421.66		
$\ln K_{\rm f} = 232.12$			$\Delta_{\mathbf{f}}G^{\circ} = \\ \ln K_{\mathbf{f}} =$		-695.98 280.75		
1 Pours 2 allower		C 11 12 C	· · · · · · · · · · · · · · · · · · ·				
1-Bromo-2-chloroethane $(1 \times C-(H)_2(C)(Cl)) + (1 \times C-(H)_2(C)(Cl))$	C)(Br))	C₂H₄BrCl					
Literature – Calculated	= Residual	Reference					
Gos abose							
Gas phase $\Delta_t H^\circ = -91.23$							
$C_p^{\circ} = 75.35$							
- 15.33							

TABLE 54. Mixed halogen compounds (18) - Continued

TABLE 54. Mixed halogen compounds (18) - Continued

	noroethylene F) ₂) + (1 × C	e C _d -(Cl)(F)), σ =	= 3	C ₂ ClF ₃	$(1 \times C_B -$	iuorobenzei $(I)(C_B)_2) + (O_B)_2$ $(I)(C_B)_2$	$(5 \times C_B - (F)(C_B)$	₂)+(4×ortho	C ₆ IF corr-(F)(F))+
	Literatur	e – Calculated =	= Residual	Reference	(4.7.2.11.1	` ` ` ` ` ` `	re – Calculated	= Residual	Reference
Gas phase									
•	-565.00	-565.00	0.00	63KOL/ZEN	Gas phase				
$C_p^{\circ} =$	83.93	83.93	0.00	53MAN/ACQ	$\Delta_{\rm f}H^{\circ} =$	-557.30	-557.40	0.10	74KRE/PRI
S° =	322.11	322.11	0.00	53MAN/ACQ	$C_p^{\circ} =$		163.20		
$\Delta_f S^\circ =$		-104.88							
$\Delta_t G^{\circ} =$		-533.73			I iauid abo				
$lnK_f =$		215.30			Liquid pha $\Delta_t H^\circ =$	– 615.20	-615.20	0.00	74VDE ODI
					$C_p^{\circ} =$	- 013.20	230.62	0.00	74KRE/PRI
					$S^{\circ} =$		332.03		
Chloropont	afluorobenz	one		C ₆ ClF ₅	$\Delta_{\mathbf{f}}S^{\circ} =$		- 267.19		
			$(4 \times orth)$	$o \operatorname{corr-}(F)(F)) +$	$\Delta_{\rm f}G^{\circ} =$		-535.54		
	corr-(F)(C)2) ((+ / 0/11/	0 (011-(1)(1)) 1	$\ln K_{\rm f} =$		216.03		
(2 \ 01110	, con-(1)(c	4))					210.05		
	Literatu	re — Calculated =	- Residual	Reference					
					1,3,5-Trich	loro-2,4,6-tı	rifluorobenzene		C ₆ Cl ₃ F
Gas phase								$(b) + (3 \times met)$	a corr-(F)(F)) +
$\Delta_t H^\circ =$	~810.00	-812.73	2.73	69COX/GUN	(3×meta	corr-(Cl)($(C1)$ + $(6 \times ortho)$	corr-(F)(Cl))
$C_p^{\circ} =$		159.83			`	` /\	,, ,	()()	•
						Literatu	re – Calculated	= Residual	Reference
Liquid pha	se								****
$\Delta_t H^\circ =$	-850.77	-851.20	0.43	69COX/GUN	Gas phase				
$C_p^{\circ} =$	221.42	220.72	0.70	68AND/COU2	$\Delta_{\rm f} H^{\circ} =$		- 528.87		
<i>s</i> ° =	300.70	326.42	-25.72	68AND/COU2	$C_p^{\circ} =$		166.29		
$\Delta_{r}S^{\circ} =$		-326.21			<u> </u>				
$\Delta_f G^\circ =$		-753.94		'					
$lnK_{\ell} =$		304.13			Liquid pha	se			
					$\Delta_t H^\circ =$		-511.20		
					$C_p^{\circ} =$		217.08		
					S° =		328.98		
	afluorobenz			C ₆ BrF ₅	$\Delta_{\mathbf{f}}S^{\circ} =$		- 343.94		
			$)_2) + (4 \times orth)$	o corr-(F)(F))+	$\Delta_i G^\circ =$		- 408.65		
(2×ortho	o corr-(F)(E	3r))	ē		$lnK_f =$		164.85		
	Literatu	re – Calculated =	= Residual	Reference					·
					Solid phase	•			
					$\Delta_f H^\circ =$		- 523.50		
Gas phase	B44 C0	#14 OF	0.25	AND POST	$C_p^{\circ} =$	197.95	196.80	1.15	73AND/MAR2
$\Delta_t H^\circ =$	-711.60	-711.85	0.25	77KRE/PRI	S° =	245.35	249.48	-4.13	73AND/MAR2
$C_p^o =$		160.15			$\Delta_{f}S^{\circ} =$		- 423.44		
			 		$\Delta_f G^\circ =$		-397.25		
Liquid sha					$lnK_f =$		160.25		
Liquid pha $\Delta_t H^\circ =$	– 754.65	- 754.90	0.25	77KRE/PRI					
•	- 134.03		0.25	//ANE/PKI					
C; = S° =		226.36 345.80							
$\Delta_t S^\circ =$		- 271.45							
$\Delta_i G^{\circ} =$		-673.97							
$\ln K_{\rm f} = -$		271.87							

TABLE 55. Summary of residuals for C-H-N-O-S-Halogen families

This table provides information on how well agreement was achieved between literature and estimated values for values of $\Delta_l H^{\circ}$ (in kJ/mol), C_p° , and S° (in J/mol·K). Residuals having $< \pm 4$ indicate good agreement, those between $> \pm 4$ and $< \pm 8$ indicate agreement in the range from fair to just acceptable, and those $> \pm 8$ suggest problems such as poor experimental data, a poor choice of group value, an unaccounted for molecular interaction, or combinations of these problems. The distribution of residuals between gas to condensed phase is about half and half. Compounds which include a ring strain correction, rsc, (such as, "cyclohexane rsc") in their molecular description and compounds which are identified by a single group, such as, methane, formaldehyde, acetonitrile, methyl bromide, etc., are excluded from this tabulation because they have zero residuals. Also excluded are compounds containing a group value in their structural group representation which was derived from a single source of thermodynamic data because such compounds will produce zero residuals. The summary of residuals is divided among the various organic families, and then summed for CH, CHO, CHN, CHNO, CHS, and organic halogen compounds as well as for all families of compounds.

Family & residual range **Properties** s° $\Delta_{\rm f}H^{\circ}$ C_p° CH Compounds n-Alkanes $< \pm 4$ 41 35 35 $> \pm 4$ to $< \pm 8$ 0 0 1 $> \pm 8$ 0 5 5 42 40 40 total t-Alkanes 35 46 34 $< \pm 4$ $> \pm 4$ to $< \pm 8$ 5 2 9 2 5 1 $> \pm 8$ 42 49 48 total q-Alkanes 27 13 22 $< \pm 4$ 3 4 9 $> \pm 4$ to $< \pm 8$ 2 $> \pm 8$ 0 0 30 24 total 26 n-Alkenes 45 34 35 $< \pm 4$ $> \pm 4$ to $< \pm 8$ 3 2 1 0 $> \pm 8$ 0 0 total 48 36 36 s-Alkenes $< \pm 4$ 36 17 20 7 5 $> \pm 4$ to $< \pm 8$ 16 $> \pm 8$ 13 2 1 65 26 26 total Alkynes 22 14 13 $< \pm 4$ $> \pm 4$ to 3 0 0 0 0 0 $> \pm 8$ 25 13 total 14

TABLE 55. Summary of residuals for C-H-N-O-S-Halogen families — Continued

Family & residual range		Properties	
· · · · · · · · · · · · · · · · · · ·	$\Delta_{\mathrm{f}}H^{\circ}$	C°	S
СН	Compounds (C	ontinued)	
Alkynes			
< ±4	22	14	1
$> \pm 4$ to	3	0	
> ±8	0	0	
otal	25	14	1
Aromat CH-01			
< ±4	54	41	3
> ±4 to < ±8	6	3	1
> ±8	5	2	
otal	65	46	. 4
Aromat CH 02			
< ±4	56	54	4
$> \pm 4$ to $< \pm 8$	15	7	1
> ±8	16	10	
otal	87	71	6
Cyclic CH-01			
< ± 4	11	12	1
$> \pm 4$ to $< \pm 8$	6 .	2	
> ±8	4	3	
otal	21	17	1
Cyclic CH-02			
< ±4	33	32	2
$> \pm 4 \text{ to } < \pm 8$	14	3	
> ±8	7	1	
otal	54	36	2
Cyclic CH-03			
< ±4	15	0	
$> \pm 4$ to $< \pm 8$	18	0	1
> ±8	20	. 0	
otal .	53	0	
Total CH cpds	$\Delta_{ m f} H^{\circ}$	C _p °	S
< ±4	375	307	25
$> \pm 4$ to $< \pm 8$	90	30	5
> ±8	67	24	2
otal	532	361	33
	СНО Сотрог	ınds	
Alcohols	· · · · · · · · · · · · · · · · · · ·		
< ±4	94	56	4:
$\Rightarrow \pm 4 \text{ to } < \pm 8$	30	5	
> ±8	19	13	
otal	143	74	5
Ethers			
< ±4	56	25	14
$\Rightarrow \pm 4 \text{ to } < \pm 8$	10	8	11
		1	. (
> ±8	11		

TABLE 55. Summary of Residuals for C-H-N-O-S-Halogen Families — Continued

TABLE 55. Summary of Residuals for C-H-N-O-S-Halogen Families - Continued

Family & residual range	Pr	operties		Family & residual range	Pro	perties	* **
	$\Delta_{\rm f} H^{\circ}$	C _P °	S°		$\Delta_t H^\circ$	C _p °	S°
СНО С	ompounds (C	ontinued)	- 		CHN Compoun	ds	
Aldehydes				Amines			
< ±4	12	10	10	< ±4	67	26	11
$> \pm 4$ to $< \pm 8$	5	0	2	> ±4 to < ±8	6	3	5
> ±8	0	7	. 5	> ±8	6	3	3
total	17	17	17	total	79	32	19
Ketones				Imines	_		
< ±4	43	14	9	< ±4	2	0	0
$> \pm$ to $< \pm 8$	4	3	3	$> \pm 4$ to $< \pm 8$	1	0	0
> ±8	1	0	2	> ±8	0	0	0
total	48	. 17	14	total	3	0	0
Acids				Nitriles			
< ±4	68	16	11	< ± 4	31	11	8
$> \pm 4$ to $< \pm 8$	25	9	0	< ±8	4	0	1
> ±8	43	3	0	$> \pm 4$ to $> \pm 8$	5	1	0
total	136	28	11	total	40	12	9
Anhydrides				Hydrazines			
< ±4	11	2	1	< ± 4	12	4	4
$> \pm 4$ to $< \pm 8$	3	0	0	$> \pm 4$ to $< \pm 8$	0	0	. 0
> ±8	4	0	0	> ±8	0	0	0
total	15	2	1	total	12	4	4
Esters				Diazenes			
< ±4	53	21	1	< ±4	14	0	0
$> \pm 4$ to $< \pm 8$	21	6	0	$> \pm 4$ to $< \pm 8$	5	0	0
> ±8	26	3	3	> ±8	1	0	. 0
total	100	30	4	total	20	0	0
Peroxides				Azides			
< ±4	7	0	0	< ±4	9	0	0
$> \pm 4$ to $< \pm 8$	0	0	0	$> \pm 4$ to $< \pm 8$	0	0	0
> ±8	3	0	0	> ±8	0	0	0
total	10	0	0	total	9	0	0
Hydroperoxides				Cyclic CHN	· · · · · · · · · · · · · · · · · · ·	 	
< ±4	4	0	0	< ±4	32	. 9	7
> ±4 to < ±8	3	0	. 0	> ±4 to < ±8	3	1	Ü
> ±8	4	0	0	> ±8	1	1	. 0
total	11	0	0	total	36	11	7
Peroxyacids		<u> </u>	······································	Total CHN cpds	$\Delta_{\rm f} H^{\circ}$	C _p °	s°
< ± 4	2	0	0			- μ	
$> \pm 4$ to $< \pm 8$	- 1	· 0	0	< ±4	167	50	30
> ±8	5	0	0	$> \pm 4$ to $< \pm 8$	19	4	6
total	8	0	0	> ±8	13	5	3
Carbonates				total	199	59	39
< ± 4	2	1	1		CHNO Compou	nds	,
> ±4 to < ±8	3	Ô	0				
> ±8	Õ	Ö	Ö	Amides			
total	5	1	1	< ± 4	22	12	. 1
				$> \pm 4$ to $< \pm 8$	3	3	Ō
Total CHO cpds	$\Delta_{\rm f} H^{\circ}$	C _p °	s°	> ±8	11	Ū-	1
				total	36	15	2
< ±4	349	145	92			 -	
$> \pm 4$ to $< \pm 8$	105	31	21				
> ±8	116 570	27 203	15 128				
total							

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TABLE 55. Summary of Residuals for C-H-N-O-S-Halogen Families — Continued

TABLE 55. Summary of Residuals for C-H-N-O-S-Halogen Families - Continued

CHNO Compounds (Continued) Family & residual range Properties CHNO Compounds (Continued) ΔμF Cc c Ureas Sulfides < ± 4 23 2 2 44 52 31 > ± 8 6 0 0 >±4 to ≤±8 3 2 >±8 > ± 8 15 0 0 >±4 to ≤±8 3 0 <th>Family & residual range</th> <th colspan="3">Properties</th> <th colspan="5">CHS Compounds (Continued)</th>	Family & residual range	Properties			CHS Compounds (Continued)				
Ucas		Δ _f H°	C_p°	S°	Family & residual ran	nge	Properties		
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	CHNC	Compounds (C	ontinued)			$\Delta_{ m f} H^{\circ}$	C _p °	S°	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Ureas				Sulfides				
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		23	2	2	< ± 4	52	31	28	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$					$> \pm 4$ to $< \pm 8$			1	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $								3	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$								32	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Amino Acids			10)1	Disulfides				
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	< ±4	28	16	5	< ±4	13	10	8	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$> \pm 4$ to $< \pm 8$	13	0	1	$> \pm 4$ to $< \pm 8$	1	0	3	
Nitroso Sulfoxides Sulfo	> ±8	5	6	5	> ±8	0	1	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	total	46	22	. 11	total	.14	11	11	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$									
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$								2	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$> \pm 4$ to $< \pm 8$	-			$> \pm 4$ to $< \pm 8$		0	0	
Nitro	> ±8				> ±8	1	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	total	8	0	. 0	total	. 8	2	2	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Nitro								
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	< ±4	65	15	6	< ± 4	27	2	2	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	< ±8	5		0	$> \pm 4$ to $< \pm 8$	15	0	0	
Nitrites and nitrates Sulfites and sulfates Sulfites and sulfites Sul	> ±8	23	2	0	> ±8	10	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	total	93	18	6	total	52	2	2	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Nitrites and nitrates						· · · · · · · · · · · · · · · · · · ·		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	< ±4						0	0	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$> \pm 4$ to $< \pm 8$	2	0	2	$> \pm 4$ to $< \pm 8$	3	. 0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	> ±8				> ±8		0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	total	17	8	_. 8	total	9	0	0	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$									
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	< ±4		0		< ± 4			3	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$								1	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	> ±8		_		> ±8			1	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	total	14	. 0	0	total	8	5	5	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$									
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$					Total CHS	$\Delta_{\mathrm{f}}H^{\circ}$	C_p°	s°	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		_	-		4	4.50			
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		-	0					73	
Total CHNO cpds $\Delta_t H^o$ C_ρ^o S^o total 198 84 $< \pm 4$ 174 52 20 Halogens $> \pm 4$ to $< \pm 8$ 29 4 3 $> \pm 8$ 53 9 6 Fluorides total 256 65 29 $< \pm 4$ 30 19 $> \pm 4$ to $< \pm 8$ 15 5 $> \pm 8$ 17 0 total 62 24 Thiols $< \pm 4$ 50 29 30 Chlorides $> \pm 4$ to $< \pm 8$ 2 2 0 $< \pm 4$ 90 49 $> \pm 8$ 0 0 2 $> \pm 4$ to $< \pm 8$ 23 7	Total	0	0	. 0				6	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Total CHNO cpds	Δ _ε H°	C _n °	s°.				5 84	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	· · · · · · · · · · · · · · · · · · ·							*****	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$						Halogens			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$					*** · 1				
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$									
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	total	256	65	29				14	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		CTIC C	•					2	
Thiols $<\pm 4$ 50 29 30 Chlorides $>\pm 4$ to $<\pm 8$ 2 2 0 $<\pm 4$ 90 49 $>\pm 8$ 0 0 2 $>\pm 4$ to $<\pm 8$ 23 7		CHS Compour	ads					6 22	
$> \pm 4$ to $< \pm 8$ 2 2 0 $< \pm 4$ 90 49 > ± 8 0 0 2 > ± 4 to $< \pm 8$ 23 7									
$> \pm 8$ 0 0 2 $> \pm 4$ to $< \pm 8$ 23 7							**		
								34	
total 52 31 32 $>+8$ 72 5								4	
	total	52	31	32	> ± 8	72	5	3 41	

TABLE 55. Summary of Residuals for C-H-N-O-S-Halogen Families — Continued

Halogens (Continued) **Bromides** 9 < ±4 > ±4 to < ±8 > ±8 total Iodides < ±4 $> \pm 4$ to $< \pm 8$ $> \pm 8$ total Mixed halogens < ±4 $> \pm 4$ to $< \pm 8$ > ±8 total Total halogens $\Delta_i H^\circ$ C_p° s° $< \pm 4$ $> \pm 4$ to $< \pm 8$ > ±8 total

TABLE 55. Summary of Residuals for C-H-N-O-S-Halogen Families — Continued

All compounds	$\Delta_{\rm f} H^{\circ}$	(%)	C_p°	(%)	S°	(%)
< ±4	1423	(67)	738	(80)	540	(76)
> ±4 to < ±8	335	(16)	91	(10)	105	(14)
> ±8	366	(17)	84	(10)	70	(10)
Grand total	2124	(100)	913	(100)	715	(100)

TABLE 56. Name and Formula Index

Name	Formula	CAS Registry No.	Family	Page
A	, , , , , , , , , , , , , , , , , , , ,		***************************************	
Acetaldehyde	C₂H₄O	75–07–0	Aldehyde	935
Acetamide	C₂H₅NO	60–35–5	Amides	1006
Acetanilide	C ₈ H ₉ NO	103-84-4	Amides	1010
Acetic acid	C ₂ H ₄ O ₂	64–19–7	Acids	945
Acetic anhydride	C ₄ H ₆ O ₃	108–24–7	Anhydrides	964
Acetone	C₃H ₆ O	67–64–1	Ketones	938
Acetonitrile'	C ₂ H ₃ N	75–05–8	Nitriles	992
Acetophenone	C_8H_8O	98–86–2	Ketones	944
Acetyl bromide	C ₂ H ₃ BrO	506–96–7	Bromide	1092
N-Acetyl-N-butylacetamide	$C_8H_{15}NO_2$	1563-86-6	Amides	1010
Acetyl chloride	C₂H₃ClO	75–36–5	Chloride	1084
Acetylene	C_2H_2	74–86–2	Alkynes	858
Acetyl fluoride	C ₂ H ₃ FO	557-99-3	Fluoride	1063
Acetyl iodide	C ₂ H ₃ IO	507-02-8	Iodide	1098
Acetylurea	$C_3H_6N_2O_2$	591–07–1	Ureas	1014
Acrylic acid	$C_3H_4O_2$	79–10–7	Acids	950
Acrylonitrile	C_3H_3N'	107–13–1	Nitriles	994
Adamantane	$C_{10}H_{16}$	281–23–2	Cyclic02	901
Adamantane-1-carboxylic acid	$C_{11}H_{16}O_2$	828-51-3	Acids	950
Adamantane-2-carboxylic acid	$C_{11}H_{16}O_2$	15897–81–1	Acids	951
1-Adamantanol	$C_{10}H_{16}O$	768-95-6	Alcohols	920
2-Adamantanol	$C_{10}H_{16}O$	700–57–2	Alcohols	920
1-Adamantyl carboxamide	$C_{11}H_{17}NO$	5511-18-2	Amides	1010
Adipic acid	$C_6H_{10}O_4$	124-04-9	Acids	952
Adiponitrile	$C_6H_8N_2$	111-69-3	Nitriles	996
DL-Alanine	C ₁ H ₂ NO ₂	302-72-7	Amino acids	1014
DL-Alanyl-DL-alanine	$C_6H_{12}N_2O_3$	2867–20–1	Amino acids	1020
DL-Alanylgiycine	$C_5H_{10}N_2O_3$	1188-01-8	Amino acids	1020
Alanylphenylalanine	$C_{12}H_{16}N_2O_3$	3061-90-3	Amino acids	1021
Allene	C₃H₄	463-49-0	n-Alkenes	851
Allenyl phenyl sulfone	C ₉ H ₈ O ₂ S	2525-42-0	Sulfones	1053
Allyl alcohol	C₃H ₆ O	107-18-6	Alcohols	909, 910
Allyl tert-butyl sulfide	C ₇ H ₁₄ S	37850-75-2	Sulfides	1047
Allylcyclohexane	C ₉ H ₁₆	2114-42-3	Cyclic02	899
Allylcyclopentane	C_8H_{14}	3524-75-2	Cyclic02	896
Allyl ethyl sulfone	C ₅ H ₁₀ O ₂ S	34008918	Sulfones	1051
Allyl ethyl sulfoxide	C ₅ H ₁₀ OS	34757-40-9	Sulfoxides	1049
Allyl methyl sulfone	$C_4H_8O_2S$	16215-14-8	Sulfones	1051
2-Aminobenzoic acid	$C_7H_7NO_2$	118-92-3	Amino acids	1018,1019
3-Aminobenzoic acid	$C_7H_7NO_2$	99-05-8	Amino acids	1019
4-Aminobenzoic acid	$C_7H_7NO_2$	150-13-0	Amino acids	1019
4-Aminohiphenyl	$C_{12}H_{11}N$	92-67-1	Amines	991
1-Aminobutane	$C_4H_{11}N$	109-73-9	Amines	983
2-Aminobutane	$C_4H_{11}N$	13952-84-6	Amines	984
4-Aminobutanoic acid	$C_4H_9NO_2$	56-12-2	Amino acids	1015
Aminoethane	C ₂ H ₇ N	75-04-7	Amines	982
Aminoethanoic acid	$C_2H_5NO_2$	56-40-6	Amino acids	1014
7-Aminoheptanoic acid	$C_7H_{15}NO_2$	929-17-9	Amino acids	1015
1-Aminohexane	$C_6H_{15}N$	111–26–2	Amines	983
2-Aminohexanoic acid	$C_6H_{13}NO_2$	616–06–8	Amino acids	1016
4-Aminohexanoic acid	$C_6H_{13}NO_2$	5415-99-6	Amino acids	1016
5-Aminohexanoic acid	$C_6H_{13}NO_2$	628-47-7	Amino acids	1016,1017
Aminomethane	CH ₅ N	74–89–5	Amines	982
2-Amino-2-methylpropane	C ₄ H ₁₁ N	75–64–9	Amines	984,985
9-Aminononanoic acid	C ₉ H ₁₉ NO ₂	1120-12-3	Amino acids	1015
1-Aminopentane	C ₅ H ₁₃ N	1120-12-3	Amines	983
5-Aminopentane 5-Aminopentanoic acid	C ₅ H ₁₁ NO ₂	660-88-8	Amino acids	1015
	C ₃ H ₁₁ NO ₂ C ₃ H ₉ N	107-10-8	Amines	982,983
1-Aminopropane				•
2-Aminopropane	C₁H₀N	75–31–0	Amines	984
DL-2-aminopropanoic Acid	C ₃ H ₇ NO ₂	302-72-7	Amino acids	1014
Aniline	C₀H ₇ N	62–53–3	Amines	989
Anisole	C ₇ II ₈ O	100-66-3	Ethers	934
Anthracene	$C_{14}H_{10} \ C_{20}H_{40}O_2$	120-12-7	Aromat02	884,885
Arachidic acid		506-30-9	Acids	949, 950

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
L-Asparagine	C ₄ H ₈ N ₂ O ₃	70-47-3	Amino acids	1018
L-Aspartic acid	$C_4H_7NO_4$	56-84-8	Amino acids	101
1-Azabicyclo[3.3.0]octane	$C_7H_{13}N$	643-20-9	CyclCHN	1000
Azelaic acid	$C_9H_{16}O_4$	123-99-9	Acids	953
Azidobenzene	$C_6H_5N_3$	622-37-7	Azides	1000
Azidocyclohexane	$C_6H_{11}N_3$	19573-22-9	Azides	1000
Azidocyclopentane	$C_5H_9N_3$	33670-50-7	Azides	1000
2-Azidoethanol	$C_2H_5N_3O$	1517-05-1	Azides	1000
Aziridine	C ₂ H ₅ N	151564	CyclCHN	1001
cis-Azobenzene	$C_{12}H_{10}N_2$	17082-12-1	Diazene	1000
trans-Azobenzene	$C_{12}H_{10}N_2$	1080166	Diazene	999,1000
Azobutane	$C_8H_{18}N_2$	2159-75-3	Diazene	999
Azo-tert-butane	$C_8H_{18}N_2$	927-83-3	Diazene	999
Azoethane	C ₄ H ₁₀ N ₂	821-14-7	Diazene	998
Azoisopropane	$C_6H_{14}N_2$	3880-49-7	Diazene	999
Azomethane	$C_2H_6N_2$	503-28-6	Diazene	998
Azopropane	$C_6H_{14}N_2$	821-67-0	Diazene	998
В				
Benzaldehyde	C_7H_6O	100-52-7	Aldehyde	938
Benzamide	C_7H_7NO	55-21-0	Amides	1010
1,2-Benzanthracene	$C_{18}H_{12}$	56553	Aromat02	886
Benzenamine	C_6H_7N	62-53-3	Amines	989
Benzene	C ₆ H ₆	71-43-2	Aromat01	863
1,2-Benzenediamine	$C_6H_8N_2$	95-54-5	Amines	991
1,3-Benzenediamine	$C_0H_8N_2$	108-45-2	Amines	991
1,4-Benzenediamine	$C_6H_8N_2$	106-50-3	Amines	991
1,2-Benzene dicarboxylic acid	C ₈ H ₆ O ₄	88-99-3	Acids	961
1,3-Benzene dicarboxylic acid	$C_8H_6O_4$	121-91-5	Acids	962
1,4-Benzene dicarboxylic acid	C ₈ H ₆ O ₄	100-21-0	Acids	962
1.2-Benzenediol	C ₆ H ₆ O ₂	120-80-9	Alcohols	924
1,3-Benzenediol	$C_6H_6O_2$	108-46-3	Alcohols	924
1,4-Benzenediol	$C_6H_6O_2$	123-31-9	Alcohols	924
Benzenemethanol	C_7H_8O	100-51-6	Alcohols	914
Benzenethiol	C6H6S	108-98-5	Thiols	1041
1,2,3-Benzene tricarboxylic acid	C ₂ H ₆ O ₆	528-44-9	Acids	962
1,3,5-Benzene tricarboxylic acid	C ₆ H ₆ O ₆	554-95-0	Acids	962
Benzil	$C_{14}H_{10}O_{2}$	134-81-6	Ketones	945
1,4-Benzodinitrile	C ₈ H ₄ N ₂	632-26-7	Nitriles	997
Benzoic acid	C ₇ H ₆ O ₂	65-85-0	Acids	956, 957
Benzoic anhydride	$C_{14}H_{10}O_3$	93-97-0	Anhydrides	
Benzonitrile	C ₇ H ₆ N	100-47-0	Nitriles	965
	• •			996
Benzophenone	$C_{i3}H_{10}O$	119-61-9	Ketones	944
Benzoyl chloride	C ₇ H ₅ ClO	98-88-4	Chloride	1084
N-Benzoylglycine	C ₉ H ₉ NO ₃	495-69-2	Amino acids	1019
Benzyl alcohol	C ₇ H ₈ O	100-51-6	Alcohols	914
Benzylamine	C ₇ H ₉ N	100-46-9	Amines	990
Benzylazide	C ₂ H ₂ N ₃	622-79-7	Azides	1000,1001
Benzyl bromide	C ₇ H ₇ Br	100-39-0	Bromide	1091
Benzyl chloride	C ₇ H ₇ Cl	100-44-7	Chloride	1073
Benzylideneaniline	$C_{i3}H_{ii}N$	538-51-2	Imines	992
Benzyl iodide	C_7H_7I	620-05-3	Iodide	1095
Benzyl mercaptan	C_7H_8S	100-53-8	Thiols	1041
Benzyl methyl sulfone	$C_8H_{10}O_2S$	3112-90-1	Sulfones	1052
Biacetyl	$C_4H_6O_2$	431-03-8	Ketones	942
9,9'-Bianthracene	$C_{28}H_{18}$	1055-23-8	Cyclic03	908
Bibenzyl	$C_{14}H_{14}$	103-29-7	Aromat02	876
Bicyclo[1.1.0]butane	C₄H ₆	157-33-5	Cyclic03	902
Bicyclobutane methyl carboxylate	$C_6H_8O_2$	4935-01-7	Esters	977
Bicyclo[2,2,1]hepta-2,5-diene	C_7H_8	121-46-0	Cyclic03	902
Bicyclo[2,2,1]heptane	C_7H_{12}	279-23-2	Cyclic03	903
Bicyclo[4.1.0]heptane	C ₇ H ₁₂ C ₇ H ₁₂	286-08-8	Cyclic03	903
Bicyclo[4.1.0]heptane Bicyclo[2,2.1]hept-2-ene		498-66-8	Cyclic03 Cyclic03	903
	C ₇ H ₁₀			
Bicycloheptyl	$C_{14}H_{26}$	23183-11-1	Cyclic03	907
Bicyclo[3,1.0]hexane	C_oH_{1o}	285_58_5	Cyclic03	902

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
Bicyclohexyl	$C_{12}H_{22}$	92–51–3	Cyclic03	907
Bicyclo[3.3.1]nonane	C_9H_{16}	280–65–9	Cyclic03	900
cis-Bicyclo[6.1.0]nonane	C_9H_{16}	13757-43-2	Cyclic03	906
trans-(+)-Bicyclo[6.1.0]nonane	C_9H_{16}	39124–79–3	Cyclic03	906
Bicyclo[2.2.2]octane	C_8H_{14}	280-33-1	Cyclic02	900
cis-Bicyclo[3.3.0]octane	C_8H_{14}	1755-05-1	Cyclic03	904
trans-Bicyclo[3.3.0]octane	C_8H_{14}	5597–89–7	Cyclic03	905
Bicyclo[4.2.0]octane	C ₈ H ₁₄	278–30–8	Cyclic03	904
Bicyclo[5.1.0]octane	C_8H_{14}	286-43-1	Cyclic03	904
Bicyclo[2.2.2]oct-2-ene	C_8H_{12}	931–64–6	Cyclic03	904
Bicyclopentyl	$C_{10}H_{18}$	1636-39-1	Cyclic02	895
Bicyclopropyl	C_6H_{10}	5685-46-1	Cyclic03	902
Bicyclo[3.3.3]undecane	$C_{11}H_{20}$	29415-95-0	Cyclic02	901
9,9'-Biphenanthrene	$C_{28}H_{18}$	20532-03-0	Cyclic03	908
Biphenyl	$C_{12}H_{10}$	92-52-4	Aromat02	877,878
2,2'-Bis(hydroxymethyl)-1,3-propanediol	$C_5H_{12}O_4$	115-77-5	Alcohol	919
2,2-Bis(4-hydroxyphenyl)-propane	$C_{15}H_{16}O_2$	80-05-7	Alcohols	925
Bis-(3,3,3-trifluoropropyl)ether	C ₆ H ₈ F ₆ O	674-65-7	Fluoride	1065
N,N-Bisuccinimide	$C_8H_8N_2O_4$	500005-58-3	CyclCHNO	1035
Bromobenzene	C ₆ H ₅ Br	108-86-1	Bromide	1091
4-Bromobenzoic acid	C ₇ H ₅ BrO ₂	586–76–5	Bromide	1091,1092
1-Bromobutane	C₄H₀Br	109-65-9	Bromide	1051,1052
2-Bromobutane	C ₄ H ₉ Br	78-76-2	Bromide	1088
1-Bromo-2-chloroethane	C₄H₄BrCl	107-04-0	Mixed	1100
1-Bromododecane	C ₁₂ H ₂₅ Br	143-15-7	Bromide	1087
Bromoethane	C_1 2 H_5 Br	74–96–4	Bromide	1087
Bromoethylene	C ₂ H ₃ Br	593-60-2	Bromide	1090
	$C_7H_{15}Br$	629-04-9	Bromide	1090
1-Bromoheptane				
1-Bromohexadecane	C ₁₆ H ₃₃ Br	112-82-3	Bromide	1087
1-Bromohexane	C ₆ H ₁₃ Br	111-25-1	Bromide	1086
Bromomethane	CH₃Br	74–83–9	Bromide	1086
1-Bromo-3-methylbutane	C ₅ H ₁₁ Br	107–82–4	Bromide	1087
1-Bromo-2-methylpropane	C ₄ H ₉ Br	78–77–3	Bromide	1087
2-Bromo-2-methylpropane	C ₄ H ₉ Br	507–19–7	Bromide	1088
1-Bromooctane	C ₈ H ₁₇ Br	111-83-1	Bromide	1087
Bromopentafluorobenzene	C ₆ BrF ₅	344-04-7	Mixed	1101
1-Bromopentane	C₅H ₁₁ Br	110-53-2	Bromide	1086
1-Bromopropane	C_3H_7Br	106-94-5	Bromide	1086
2-Bromopropane	C_3H_7Br	75–26–3	Bromide	1088
1-Bromo-1-propene (E)	C₃H₅Br	590–15–8	Bromide	1090
1-Bromo-1-propene (Z)	C ₃ H ₅ Br	590-13-6	Bromide	1090
3-Bromo-1-propene	C ₃ H ₅ Br	106–95–6	Bromide	1090
1-Bromopropyne	C_3H_3Br	2003-82-9	Bromide	1090
1,2-Butadiene	C_4H_6	590-19-2	n-Alkenes	850
1,3-Butadiene	C_4H_6	106–99–0	n-Alkenes	850
Butadiync	C ₄ H ₂	460 12 8	Alkynes	861
Butanal	C_4H_8O	123-72-8	Aldehyde	936
Butanamide	C ₄ H ₉ NO	541-35-5	Amides	1007
Butane	C_4H_{10}	106–97–8	n-Alkanes	830
Butanediamide	C ₄ H ₈ N ₂ O ₂	110–14–5	Amides	1010
1.2-Butanediamine	$C_4H_{12}N_2$	4426–48–6	Amines	984
1,4-Butanedinitrile	C ₄ H ₄ N ₂	110-61-2	Nitriles	996
Butanedioic acid	C ₄ H ₆ O ₄	110-15-6	Acids	951
1,2-Butanediol	$C_4H_{10}O_2$	584-03-2	Alcohols	918
•				918
1,3-Butanediol	$C_4H_{10}O_2$	107-88-0	Alcohols	
1,4-Butanediol	$C_4H_{10}O_2$	110-63-4	Alcohols	918
2,3-Butanediol	$C_4H_{10}O_2$	513-85-9	Alcohols	918
2,3-Butanedione	$C_4H_6O_2$	431–03–8	Ketones	942
1,4-Butanedithiol	$C_4H_{10}S_2$	1191088	Thiols	1038
Butanenitrile	C_4H_7N	109–74–0	Nitriles	992,993
1,2,3,4-Butanetetrol	$C_4H_{10}O_4$	149–32–6	Alcohols	919
1-Butanethiol	$C_4H_{10}S$	109-79-5	Thiols	1036
2-Butanethiol	$C_4H_{10}S$	513-53-1	Thiols	1038
Butanoic acid	$C_4H_8O_2$	107-92-6	Acids	946
Butanol	$C_4H_{10}O$	71–36–3	Alcohols	910

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
4-Butanolactone	C₄H ₆ O ₂	96-48-0	Esters	97:
Butanone	C₄H ₈ O	78–93–3	Ketones	938
Butanoyl chloride	C₄H₁ClO	141-75-3	Chloride	1084
trans-2-Butenal	C4H6O	4170-30-3	Aldehyde	930
1-Butene	C₄H ₈	106-98-9	n-Alkenes	846
cis-2-Butene	C_4H_8	590-18-1	n-Alkenes	847
trans-2-Butene	C_4H_8	624-64-6	n-Alkenes	848
(E)-2-Butenedioic acid	C ₄ H ₄ O ₄	110-17-8	Acids	951
(Z)-2-Butenedioic acid	C ₄ H ₄ O ₄	110-16-6	Acids	951
cis-2-Butenenitrile	C ₄ H ₅ N	1190-76-7	Nitriles	994
trans-2-Butenenitrile	C ₄ H ₅ N	627-26-9	Nitriles	994
1-Buten-3-yne	C ₄ H ₄	689-97-4	Alkynes	861
Butoxybutane	C ₈ H ₁₈ O	142–96–1	Ethers	927
2-Butoxy-2-butane	C ₈ H ₁₈ O	6863–58–7	Ethers	928
Butoxyethene	C₀H₁₂O	111-34-2	Ethers	929
N-Butylacetamide	C ₆ H ₁₃ NO	1119-49-9	Amides	1009
N-tert-Butylacetamide	C₀H₁₃NO	762-84-5	Amides	1009
Butyl acetate	$C_6H_{12}O_2$	123-86-4	Esters	969
tert-Butyl acetate	C ₆ H ₁₂ O ₂	540–88–5	Esters	970
n-Butyl alcohol	CH10O	71-36-3	Alcohols	910
sec-Butyl alcohol	C₄H ₁₀ O	78-92-2	Alcohols	915
tert-Butyl alcohol	C ₄ H ₁₀ O	75-65-0	Alcohols	916
n-Butyl amine	C ₄ H ₁₁ N	109-73-9	Amines	983
sec-Butyl amine	C ₄ H ₁₁ N	13952-84-6	Amines	984
tert-Butyl amine	C ₄ H ₁₁ N	75-64-9	Amines	984,985
Butylbenzene	C ₁₀ H ₁₄	104-51-8	Aromat01	866
sec-Butylbenzene	C ₁₀ H ₁₄ C ₁₀ H ₁₄	135-98-8	Aromat02	872
tert-Butylbenzene		98-06-6	Aromat02	873
Butyl (E)-2-butenoate	C ₈ H ₁₄ O ₂	7299-91-4	Esters	973
Butyl trans-2-butenoate Butyl chloroacetate	C ₈ H ₁₄ O ₂	7299-91-4	Esters	973
Butyl 2-chlorobutanoate	C ₆ H ₁₁ ClO ₂ C ₈ H ₁₅ ClO ₂	590-02-3 62108-74-1	Chloride	1081
Butyl 2-chloropropanoate		54819-86-2	Chloride	1083
Butyl 3-chloropropanoate	C ₇ H ₁₃ ClO ₂		Chloride	1082
Butylcyclohexane	C ₇ H ₁₃ ClO ₂ C ₁₀ H ₂₀	27387-79-7 1678-93-9	Chloride	1082
Butylcyclonexane	C ₁₀ H ₁₈		Cyclic02	898
N-Butyldiacetamide	C ₈ H ₁₅ NO ₂	2040-95-1 1563-86-6	Cyclic02	893
N-Butyldiacetylamine	C ₈ H ₁₅ NO ₂	1563-86-6	Amides	1009
Butyl dichloroacetate			Amides	1009
N-Butylethanamide	C ₆ H ₁₀ Cl ₂ O ₂ C ₆ H ₁₃ NO	29003-73-4 1119-49-9	Chloride Amides	1083
Butyl ethanoate	C ₆ H ₁₂ O ₂	123-86-4	Esters	1009
Butyl ethyl sulfide	C ₆ H ₁₄ S	638-46-0		969
tert-Butyl ethyl sulfide	C ₆ H ₁₄ S	14290-92-7	Sulfides Sulfides	1042,1043
tert-Butyl ethyl sulfone	C ₆ H ₁₄ O ₂ S	34008-94-1	Sulfones	1047
tert-Butyl ethyl sulfoxide	C ₆ H ₁₄ OS	25432-20-6	Sulfoxides	1051
Butyl heptyl sulfide	C ₁₁ H ₂₄ S	40813-84-1		1050
tert-Butyl hydroperoxide	C ₄ H ₁₀ O ₂	75-91-2	Sulfides	1045
n-Butylisobutylamine	C ₈ H ₁₉ N	20810-06-4	Hydroperoxides	979
N-Butylisobutyleneimine	C ₈ H ₁₇ N	6898-75-5	Amines	986
Butyl methyl sulfide	C ₅ H ₁₂ S	628-29-5	Imines	992
tert-Butyl methyl sulfide	C ₅ H ₁₂ S		Sulfides	1042
Butyl methyl sulfone	C ₅ H ₁₂ O ₂ S	6163-64-0 7560-59-0	Sulfides	1046
tert-Butyl methyl sulfone	C ₃ H ₁₂ O ₂ S	14094-12-3	Sulfones	1051
1-Butyinaphthalene	C ₁₄ H ₁₆	1634-09-9	Sultones A	1051
2-Butylnaphthalene	C ₁₄ H ₁₆	1134-62-9	Aromat02	881
Butyl nonyl sulfide	C ₁₃ H ₂₈ S		Aromat02	881
Butyl pentadecyl sulfide	C ₁₉ H ₄₀ S	66577-32-0 66359-42-0	Sulfides	1046
N-Butylpentanamide	C ₁ 9H ₄₀ S C ₉ H ₁₉ NO	66359~42~0	Sulfides	1046
Butyl pentanoate		2763-67-9	Amides	1009
Butyl pentanoate tert-Butyl perdecanoate	C ₉ H ₁₈ O ₂	591-68-4	Esters	970
	C ₁₄ H ₂₈ O ₃	16474-36-5	Peroxyacids	981
tert-Butyl perdodecanoate	C ₁₆ H ₃₂ O ₃	2123-88-8	Peroxyacids	981
tert-Butyl pertetradecanoate	C ₁₈ H ₃₆ O ₃	59710-71-3	Peroxyacids	981
Butyl propyl sulfide	C ₇ H ₁₆ S	1613-46-3	Sulfides	1043
tert-Butyl-(1,1,3,3-tetramethylbutyl)diazene	$C_{12}H_{26}N_2$	57905-89-2	Diazene	999
N-n-Butylurea N-sec-Butylurea	$C_5H_{12}N_2O$ $C_2H_{12}N_2O$	592-31-4	Ureas	1012
		689-11-2	Ureas	1012

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
N-tert-Butylurea	C ₅ H ₁₂ N ₂ O	1118–12–3	Ureas	1012
Butyl valerate	$C_9H_{18}O_2$	591684	Esters	970
n-Butyl vinyl ether	$C_6H_{12}O$	111-34-2	Ethers	929
1-Butyne	C_4H_6	107006	Alkynes	858
2-Butyne	C_4H_6	503–17–3	Alkynes	860
2-Butyne-1,4-dinitrile	C_4N_2	1071–98–3	Nitriles	996
Butyraldehyde	C₄H ₈ O	123-72-8	Aldehyde	936
Butyramide	C ₄ H ₉ NO	541-35-5	Amides	1007
Butyric acid	$C_4H_8O_2$	107–92–6	Acids	946
τ-Butyrolactone	$C_4H_6O_2$	96-48-0	Esters	975
Butyronitrile	C ₄ H ₇ N	109–74–0	Nitriles	992,993
С				
Capric acid	$C_{10}H_{20}O_2$	334–48–5	Acids	947
Caprinitrile	$C_{10}H_{19}N$	1975–78–6	Nitriles	993
Caproic acid	$C_6H_{12}O_2$	142-62-1	Acids	946
Caprolactone	$C_6H_{10}O_2$	502-44-3	Esters	975
Caprylic acid	$C_8H_{16}O_2$	124-07-2	Acids	947
Capryonitrile	$C_8H_{15}N$	124–12–9	Nitriles	993
Catechol	$C_6H_6O_2$	120-80-9	Alcohols	924
Cetyl alcohol	$C_{16}H_{34}O$	36653-82-4	Alcohois	913
Chloroacetic acid	$C_2H_3ClO_2$	79–11–8	Chloride	1079
Chloroacetyl chloride	$C_2H_2Cl_2O$	79-04-9	Chloride	1084
2-Chlorobenzaldehyde	C ₇ H₅ClO	89-98-5	Chloride	1080
3-Chlorobenzaldehyde	C ₇ H ₅ ClO	587-04-2	Chloride	1080
4-Chlorobenzaldehyde	C ₇ H₅ClO	104-88-1	Chloride	1081
Chlorobenzene	C ₆ H ₅ Cl	108–90–7	Chloride	1072
2-Chloro-1,4-benzenediol	$C_6H_5ClO_2$	615–67–8	Chloride	1078
2-Chlorobenzoic acid	C ₇ H ₅ ClO ₂	118-91-2	Chloride	1080
3-Chlorobenzoic acid	C ₇ H ₅ ClO ₂	535-80-8	Chloride	1080
4-Chlorobenzoic acid	C7H5ClO2	74-11-3	Chloride	1080
2-Chlorobenzoyl chloride	C ₇ H₄Cl ₂ O	609–65–4	Chloride	1085
3-Chlorobenzoyl chloride	C₂H₄Cl₂O	618-46-2	Chloride	1085
4-Chlorobenzoyl chloride	C ₇ H ₄ Cl ₂ O	122-01-0	Chloride	1085
1-Chlorobutane	C ₄ H ₉ Cl	109-69-3	Chloride	1066
2-Chlorobutane	C₄H ₉ Cl	78864	Chloride	1067
2-Chlorobutanoic acid	C ₄ H ₇ ClO ₂	4170–24–5	Chloride	1079
3-Chlorobutanoic acid	C ₄ H ₇ ClO ₂	1951–12–8	Chloride	1079
4-Chlorobutanoic acid	C ₄ H ₇ ClO ₂	627-00-9	Chloride	1079
Chlorocyclohexane	C₀H₁₁Cl	542–18–7	Chloride	1076
1-Chloro-1,1-difluoroethane	$C_2H_3ClF_2$	75-68-3	Mixed	1100
1-Chlorododecane	$C_{12}H_{25}CI$	112–52–7	Chloride	1067
Chloroethane	C₂H₅Cl	75003	Chloride	1066
1-Chloro-2-ethoxyethane	C ₄ H ₉ ClO	628-34-2	Chloride	1081
(1-Chloroethyl)benzene	C ₈ H ₉ Cl	672-65-1	Chloride	1073
1-Chloro-2-ethylbenzene	C ₈ H ₉ Cl	89-96-3	Chloride	1073
1-Chloro-4-ethylbenzene	C₅H₀Cl	622–98–0	Chloride	1073
Chloroethylene	C₂H₃Cl	75-01-4	Chloride	1071
2-Chloroethyl vinyl ether	C₄H₁ClO	110-75-8	Chloride	1081
1-Chloro-1-fluoroethane	C₂H₄CIF	1615-75-4	Mixed	1099
2-Chlorohexane	C ₆ H ₁₃ Cl	638-28-8	Chloride	1068
Chloromethane	CH₃Cl	74-87-3	Chloride	1066
1-Chloro-4-methylbenzene	C ₇ H ₇ Cl	106-43-4	Chloride	1072,1073
1-Chloro-3-methylbutane	C ₅ H ₁₁ Cl	107-84-6	Chloride	1067
2-Chloro-2-methylbutane	C₅H ₁₁ Cl	594-36-5	Chloride	1068
2-Chloro-3-methylbutane	C ₅ H ₁₁ Cl	631-65-2	Chloride	1068
1-Chloro-2-methylpropane	C ₄ H ₉ Cl	513-36-0	Chloride	1067
2-Chloro-2-methylpropane	C ₄ H ₉ Cl	507-20-0	Chloride	1068
1-Chloronaphthalene	C ₁₀ H ₇ Cl	90-13-1	Chloride	1073
2-Chloronaphthalene	$C_{10}H_7Cl$	91–58–7	Chloride	1074
1-Chlorooctadecane	$C_{18}H_{37}Cl$	3386–33–2	Chloride	1067
1-Chlorooctane	C ₈ H ₁₇ Cl	111-85-3	Chloride	1066
Chloropentafluorobenzene	C ₆ CIF ₅	344-07-0	Mixed	1101
1-Chloro-1,1,3,3,3-pentafluoropropane	C ₃ H ₂ ClF ₅	460-92-4	Mixed	1099
		TUU-74-T	DOVITE	1077
1-Chloropentane	C₅H ₁₁ Cl	543-59-9	Chloride	1066

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
3-Chlorophenol	C ₆ H₅ClO	108-43-0	Chloride	1076
4-Chlorophenol	C ₆ H ₅ ClO	106-48-9	Chloride	1076
1-Chloropropane	C_3H_7Cl	540-54-5	Chloride	1066
2-Chloropropane	C₃H ₇ Cl	75–29–6	Chloride	1067
3-Chloro-1,2-propanediol	$C_3H_7ClO_2$	96-24-2	Chloride	1076
2-Chloro-1,3-propanediol	C₃H7ClO2	497-04-1	Chloride	1076
2-Chloropropanoic acid	$C_3H_5ClO_2$	598-78-7	Chloride	1079
3-Chloropropanoic acid	C₃H₅ClO₂	107-94-8	Chloride	1079
2-Chloro-1-propene	C₃H₅Cl	557-98-2	Chloride	1071
3-Chloro-1-propene	C₃H₅Cl	107-05-1	Chloride	1071
1-Chloropropyne	C ₃ H ₃ Cl	7747-84-4	Chloride	1072
p-Chlorotoluene	C ₂ H ₂ Cl	106-43-4	Chloride	1072,1073
Chlorotrifluoroethylene	C ₂ ClF ₃	79-38-9	Mixed	1101
1-Chloro-3,3,3-trifluoropropane	C ₃ H ₄ ClF ₃	460-35-5	Mixed	1100
Chrysene	$C_{18}H_{12}$	218-01-9	Aromat02	885
Coronene	$C_{24}H_{12}$	191-07-1	Aromat02	886
m-Cresol	C ₇ H ₈ O	108-39-4	Alcohols	921
o-Cresol	C ₇ H ₈ O	95–48–7	Alcohols	921
	C ₇ H ₈ O	106-44-5	Alcohols	921
p-Cresol	C₁H ₆ O	4170–30–3		
Crotonaldehyde		277-10-1	Aldehyde	936
Cubane	C_8H_8		Cyclic03	904
Cubane 1,4-dimethyldicarboxylate	$C_{12}H_{12}O_4$	29412–62–2	Esters	977
Cumene	C ₉ H ₁₂	92–82–8	Aromat02	872
Cumyl hydroperoxide	$C_0H_{12}O_2$	80-15-9	Hydroperoxides	980
Cyclobutane	C₄H ₈	287-23-0	Cyclic01	887
Cyclobutane-1,3-dione	C ₄ H ₄ O ₂	15506–53–3	Ketones	945
Cyclobutane Methyl Carboxylate	$C_6H_{10}O_2$	765–85–5	Esters	977
Cyclobutanenitrile	C _s H ₂ N	4426-11-3	Nitriles	995
Cyclobutene	C_4H_6	822-35-5	Cyclic01	889
Cyclobutylamine	C_4H_9N	2516-34-9	Amines	988
Cyclodecane	$C_{10}H_{20}$	293-96-9	Cyclic01	888
Cyclodecanone	$C_{10}H_{18}O$	1502063	Ketones	943
Cyclododecane	$C_{12}H_{24}$	294-62-2	Cyclic01	888
Cyclododecanone	$C_{12}H_{22}O$	830–13–7	Ketones	943
Cycloheptadecane	$C_{17}H_{34}$	295-97-6	Cyclic01	888
Cycloheptadecanone	$C_{17}H_{32}O$	3661-77-6	Ketones	943
1,3-Cycloheptadiene	C_7H_{10}	4054-38-0	Cyclic01	890
Cycloheptane	C ₇ H ₁₄	291-64-5	Cyclic01	887
Cycloheptanol	$C_7H_{14}O$	502-41-0	Alcohols	920
Cycloheptanone	$C_7H_{12}O$	502-42-1	Ketones	942
1,3,5-Cycloheptatriene	C_7H_8	544-25-2	Cyclic01	890
Cycloheptene	C_7H_{12}	628-92-2	Cyclic01	889
Cycloheptyl alcohol	C ₇ H ₁₄ O	502-41-0	Alcohols	920
Cyclohexadecane	C ₁₆ H ₃₂	295-65-8	Cyclic01	888
1,3-Cyclohexadiene	C_6H_8	592–57–4	Cyclic01	889,890
1,4-Cyclohexadiene	C ₆ H ₈	628-41-1		-
Cyclohexane	C ₆ H ₁₂	110-82-7	Cyclic01 Cyclic01	890
-	$C_7H_{11}N$		-	887
Cyclohexanenitrile		766-05-2	Nitriles	995
Cyclohexanethiol	C ₆ H ₁₂ S	1569-69-3	Thiols	1040
Cyclohexanol	C₄H ₁₂ O	108-93-0	Alcohols	920
Cyclohexanone	C₅H ₁₀ O	108-94-1	Ketones	942
Cyclohexene	C ₆ H ₁₀	110-83-8	Cyclic01	889
Cyclohexyl alcohol	$C_6H_{12}O$	108–93–0	Alcohols	920
Cyclohexylamine	$C_6H_{13}N$	108-91-8	Amines	989
3-Cyclohexyleicosane	$C_{26}H_{52}$	4443–57–6	Cyclic02	899
9-Cyclohexyleicosane	$C_{26}H_{52}$	4443-61-2	Cyclic02	899
11-Cyclohexylheneicosane	$C_{27}H_{54}$	6703-99-7	Cyclic02	899
13-Cyclohexylpentacosane	$C_{31}H_{62}$	6697–15–0	Cyclic02	900
Cyclononane	C ₉ H ₁₈	293-55-0	Cyclic01	888
Cyclononanone	C ₀ H ₁₆ O	3350-30-9	Ketones	943
1,5-Cyclooctadiene	C_8H_{12}	111-78-4	Cyclic01	890
Cyclooctane	C ₈ H ₁₆	292-64-8	Cyclic01	887
Cyclooctane	C ₈ H ₁₄ O	502-49-8	Ketones	943
Cyclooctatetraene				
	C_8H_8	629-20-9	Cyclic01	890
Cyclooctene	C ₈ H ₁₄	931-88-4	Cyclic01	889
Cyclopentadecane	$C_{15}H_{30}$	295-48-7	Cyclic01	888

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
Cyclopentadecanone	C ₁₅ H ₂₈ O	502-72-7	Ketones	943
,3-Cyclopentadiene	C₅H ₆	542-92-7	Cyclic01	889
Cyclopentane	C_5H_{10}	287-92-3	Cyclic01	887
Cyclopentanenitrile	C₀H₀N	4254-02-8	Nitriles	995
Cyclopentanethiol	C₅H ₁₀ S	1679-07-8	Thiols	1039
Cyclopentanol	C₅H ₁₀ O	96-41-3	Alcohols	920
yclopentanone	C₅H ₈ O	120-92-3	Ketones	942
Cyclopentene	C ₅ H ₈	142–29–0	Cyclic01	889
Cyclopentyl alcohol	$C_5H_{10}O$	96-41-3	Alcohols	920
Cyclopentyl anconor Cyclopentylamine	$C_5H_{11}N$	1003-03-8	Amines	989
Cyclopentylcycloheptane	$C_{12}H_{22}$	42347-48-8	Cyclic03	907
Cyclopentylcyclohexane	$C_{12}H_{22}$ $C_{11}H_{20}$	1606-08-2	•	
			Cyclic03	906,907
1-Cyclopentylheneicosane	$C_{26}H_{52}$	6703–81–7	Cyclic02	895
Cyclopentyl methyl sulfide	C ₆ H ₁₂ S	7133–36–0	CyclCHS	1057
-Cyclopentyl-1-propene	C ₈ H ₁₄	3524-75-2	Cyclic02	896
Cyclopropane	C_3H_6	75–19–4	Cyclic01	887
Cyclopropanenitrile	C₄H₅N	5500-21-0	Nitriles	995
Cyclopropene	C₃H₄	2781-85-3	Cyclic01	889
Cyclopropylamine	C_3H_7N	765–30–0	Amines	988
Cyclotetradecane	$C_{14}H_{28}$	295-17-0	Cyclic01	888
,3,5,7-Cyclotetramethylenetetranitramine	$C_4H_8N_8O_8$	2691-41-0	Nitramines	1034
Cyclotridecane	$C_{13}H_{26}$	295-02-3	Cyclic01	888
1,3,5-Cyclotrimethylenetrinitramine	C ₃ H ₆ N ₆ O ₆	121-82-4	Nitramines	1034
1,3,5-Cyclotrimethylenetrinitrosamine	$C_3H_6N_6O_3$	13980-04-6	Nitroso	1022
Cycloundecane	$C_{11}H_{22}$	294–41–7	Cyclic01	888
Cycloundecanone	$C_{11}H_{20}O$	878–13–7	Ketones	943
D	C111120C	070-137	Retories	<i>3</i> 43
		404.00.0		
Decafluorobiphenyl	$C_{12}F_{10}$	434–90–2	Fluoride	1060
Decaldehyde	$C_{10}H_{20}O$	112–31–2	Aldehyde	937
is-Decalin	$C_{10}H_{18}$	493-01-6	Cyclic02	900
rans-Decalin	$C_{10}H_{18}$	493–02–7	Cyclic02	900
Decanal	$C_{10}H_{20}O$	112-31-2	Aldehyde	937
Decane	$C_{10}II_{22}$	124-18-5	n-Alkanes	831
Decanedioic acid	$C_{10}H_{18}O_4$	111–20–6	Acids	953
1,10-Decanediol	$C_{10}H_{22}O_2$	112-47-0	Alcohols	919,920
Decanenitrile	$C_{10}H_{19}N$	1975–78–6	Nitriles	993
1-Decanethiol	C ₁₀ H ₂₂ S	143-10-2	Thiols	1037
Decanoic acid	$C_{10}H_{20}O_2$	334-48-5	Acids	947
Decanol	$C_{10}H_{22}O$	112-30-1	Alcohols	911
1-Decene	$C_{10}H_{20}$	872-05-9	n-Alkenes	847
cis-3-Decen-1-yne	C ₁₀ H ₁₆	61827–88–1	Alkynes	861
trans-3-Decen-1-yne	$C_{10}H_{16}$	2807-10-5	Alkynes	861
n-Decyl alcohol	C ₁₀ H ₁₆ C ₁₀ H ₂₂ O	112-30-1	Alcohols	911
		104-72-3		
Decylbenzene	$C_{16}H_{26}$ $C_{15}H_{30}$		Aromat01	867 894
Decylcyclopentane		1795-21-7	Cyclic02	
1-Decyne	$C_{10}H_{18}$	764–93–2	Alkynes	859,860
Diacetyl	$C_4H_6O_2$	431–03–8	Ketones	942
Diacetyl peroxide	$C_4H_6O_4$	110–22–5	Peroxide	978
Dibenzoylmethane	$C_{15}H_{12}O_2$	120-46-7	Ketones	945
Dibenzoyl peroxide	$C_{14}H_{10}O_4$	94-36-0	Peroxide	978
Dibenzyl sulfone	$C_{14}H_{14}O_2S$	620-32-6	Sulfones	1054
1,2-Dibromobutane	$C_4H_8Br_2$	533-98-2	Bromide	1088
1,3-Dibromobutane	C ₄ H ₈ Br ₂	107-80-2	Bromide	1089
1,4-Dibromobutane	$C_4H_8Br_2$	110-52-1	Bromide	1089
2,3-Dibromobutane	$C_4H_8Br_2$	5408-86-6	Bromide	1089
1,2-Dibromocycloheptane	$C_7H_{12}Br_2$	29974-68-3	Bromide	1091
1,2-Dibromocyclohexane	$C_6H_{10}Br_2$	5401-62-7	Bromide	1091
1,2-Dibromocyclooctane	C ₈ H ₁₄ Br ₂	29974-69-4	Bromide	1091
1,2-Dibromocyclopentane	C ₅ H ₈ Br ₂	10230-26-9	Bromide	1091
1,2-Dibromo-1,2-dichloroethane	$C_2H_2Br_2Cl_2$	683-68-1	Mixed	1099
1,2-Dibromoethane	$C_2H_4Br_2$	106–93–4	Bromide	1088
1,2-Dibromoheptane	$C_7H_{14}Br_2$	42474-21-5	Bromide	1089
2,3-Dibromo-2-methylbutane	$C_5H_{10}Br_2$	594–51–4	Bromide	1089,1090
1,2-Dibromo-2-methylpropane			Bromide	

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
1,2-Dibromopropane	C₃H ₆ Br ₂	78–75–1	Bromide	1088
1,3-Dibromopropane	$C_3H_6Br_2$	109-64-8	Bromide	1089
1,2-Dibromotetrafluoroethane	C ₂ Br ₂ F ₄	124-73-2	Mixed	1099
Dibutanoyl peroxide	C ₈ H ₁₄ O ₄	2697-95-2	Peroxide	978
Di-n-butylamine	C ₈ H ₁₉ N	111-92-2	Amines	986
Di-n-butyldiazene	$C_8H_{18}N_2$	2159-75-3	Diazene	999
Di-tert-hutyldiazene	C ₈ H ₁₈ N ₂	927-83-3 87339-11-5	Diazene Nitroso	999
Di-tert-butyldiazene N-oxide (E)	$C_8H_{18}N_2O$ $C_8H_{18}S_2$	629-45-8	Disulfides	1022 1048
Di-n-butyl disulfide	C ₈ H ₁₈ O ₂ C ₈ H ₁₈ O	142-96-1	Ethers	927
Di-n-butyl ether Di-sec-butyl ether	$C_8H_{18}O$	6863-58-7	Ethers	927
Di-tert-butyl ether	$C_8H_{18}O$	6163-66-2	Ethers	929
Di-n-butyl ketone	C ₈ H ₁₈ O	502–56–7	Ketones	939,940
Di-tert-butyl ketone	C ₉ H ₁₈ O	815–24–7	Ketones	941
Di-tert-butyl peroxide	$C_8H_{18}O_2$	110-05-4	Peroxide	978
Di-n-butyl sulfate	$C_8H_{18}O_4S$	625-22-9	Sulfates	1055
Di-n-butyl sulfide	$C_8H_{18}S$	544-40-1	Sulfides	1044,1045
Di-tert-butyl sulfide	$C_8H_{18}S$	107-47-1	Sulfides	1044
Di-n-butyl sulfite	C ₈ H ₁₈ O ₂ S	626-85-7	Sulfites	1055
Di-tert-butyl sulfone	$C_8H_{18}O_2S$	1886–75–5	Sulfones	1051
Di-n-butyl sulfone	$C_8H_{18}O_2S$	598-04-9	Sulfones	1052
N,N'-(Di-tert-butyl)urea	$C_9H_{20}N_2O$	5336-24-3	Ureas	1013
Dibutyryl peroxide	C _R H ₁₄ O ₄	2697-95-2	Peroxide	978
Dichloroacetic acid	$C_2H_2Cl_2O_2$	79-43-6	Chloride	1080
Dichloroacetyl chloride	C ₂ HCl ₃ O	79–36–7	Chloride	1084
1,2-Dichlorobenzene	$C_6H_4Cl_2$	95-50-1	Chloride	1074
1,3-Dichlorobenzene	$C_6H_4Cl_2$	541-73-1	Chloride	1074
1,4-Dichlorobenzene	$C_6H_4Cl_2$	106-46-7	Chloride	1074
2,3-Dichloro-1,4-benzenediol	C ₆ H ₄ Cl ₂ O ₂	608-44-6	Chloride	1077
2,5-Dichloro-1,4-benzenediol	C ₆ H ₄ Cl ₂ O ₂	824-69-1	Chloride	1077
2,6-Dichloro-1,4-benzenediol	C ₆ H ₄ Cl ₂ O ₂	20103-10-0	Chloride	1077
2,2'-Dichlorobiphenyl	C ₁₂ H ₈ Cl ₂	13029-08-8	Chloride	1075
4,4'-Dichlorobiphenyl	C ₁₂ H ₈ Cl ₂	2050–68–2	Chloride	1075
1,1-Dichloroethane	C ₂ H ₄ Cl ₂ C ₂ H ₄ Cl ₂	75–34–3	Chloride	1069
1,2-Dichloroethane 1,1-Dichloroethylene	$C_2H_2Cl_2$	107062 75354	Chloride Chloride	1068 1071
1,2-Dichloroethylene (E)	$C_2H_2Cl_2$ $C_2H_2Cl_2$	156-59-2	Chloride	1071
1,2-Dichloroethylene (Z)	C ₂ H ₂ Cl ₂	156-60-5	Chloride	1071
1,2-Dichloropropane	C ₃ H ₆ Cl ₂	78–87–5	Chloride	1068
1,3-Dichloropropane	C ₃ H ₆ Cl ₂	142-28-9	Chloride	1069
2,2-Dichloropropane	C ₃ H ₆ Cl ₂	594-20-7	Chloride	1069
1,3-Dichloro-2-propanol	C ₃ H ₆ Cl ₂ O	96-23-1	Chloride	1077
2,3-Dichloro-1-propanol	C ₃ H ₆ Cl ₂ O	616-23-9	Chloride	1077
2,5-Dichlorostyrene	C ₈ H ₆ Cl ₂	1123-84-8	Chloride	1075
1,2-Dichlorotetrafluoroethane	$C_2Cl_2F_4$	76-14-2	Mixed	1099
3,3-Dichloro-1,1,1-trifluoropropane	$C_3H_3Cl_2F_3$	460-69-5	Mixed	1099
1,4-Dicyanatobenzene	$C_8H_4N_2O_2$	3729-34-8	Nitroso	1022
1,4-Dicyanobenzene	$C_8H_4N_2$	623-26-7	Nitriles	997
1,4-Dicyanobenzene di-N-oxide	$C_8H_4N_2O_2$	3729-34-8	Nitroso	1022
Dicyclopentylmethane	$C_{11}H_{20}$	2619-34-3	Cyclic03	907
Di-n-decyl disulfide	$C_{20}H_{42}S_2$	10496-18-1	Disulfides	1049
1,1-Diethoxyethane	$C_6H_{14}O_2$	105-57-7	Ethers	930
1,2-Diethoxyethane	$C_6H_{14}O_2$	629-14-1	Ethers	930
Diethoxymethane	$C_5H_{12}O_2$	462-95-3	Ethers	930
1,3-Diethoxypropane	$C_7H_{16}O_2$	3459-83-4	Ethers	931
2,2-Diethoxypropane	$C_7H_{16}O_2$	126-84-1	Ethers	931
Diethylamine	$C_4H_{11}N$	109-89-7	Amines	985
1,2-Diethylbenzene	$C_{10}H_{14}$	135-01-3	Aromat01	870
1,3-Diethylbenzene	$C_{10}H_{14}$	141–93–5	Aromat01	871
1,4-Diethylbenzene	$C_{10}H_{14}$	105-05-5	Aromat01	871
3,5-Diethylbenzoic acid	$C_{11}H_{14}O_2$	3854–90–5	Acids	961
Diethyl butanedioate	C ₈ H ₁₄ O ₄	123-25-1	Esters	974,975
2,2-Diethyl-1,4-butanedioic acid	C ₈ H ₁₄ O ₄	5692–97–7	Acids	955
meso-2,3-Diethyl-1,4-butanedioic acid	C ₈ H ₁₄ O ₄	35392-80-4	Acids	954
racemic-2,3-Diethyl-1,4-butanedioic acid	C ₈ H ₁₄ O ₄	35392-77-9	Acids	954,955
Diethyl carbonate	$C_5H_{10}O_3$	105-58-8	Carbonates	982

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
cis-1,2-Diethylcyclopropane	C ₇ H ₁₄	1192-18-3	Cyclic03	90
rans-1,2-Diethylcyclopropane	C7H14	822-50-4	Cyclic03	90
Diethyldiazene	$C_4H_{10}N_2$	821-14-7	Diazene	99
Diethyl disulfide	$C_4H_{10}S_2$	110-81-6	Disulfides	104
V,N'-Diethyl-N,N'-diphenylurea	C ₁₇ H ₂₀ N ₂ O	85-98-3	Ureas	101
Diethylene glycol	$C_4H_{10}O_3$	111-46-6	Ethers	93
Diethyl ethanedioate	$C_6H_{10}O_4$	95-92-1	Esters	97
Diethyl ether	C ₄ H ₁₀ O	60-29-7	Ethers	92
Diethyl ketone	C ₅ H ₁₀ O	9622-0	Ketones	93
Diethyl malonate	$C_7H_{12}O_4$	105-53-3	Esters	97-
Diethylnitramine	$C_4H_{10}N_2O_2$	7119–92–8	Nitramines	103
Diethyl oxalate	$C_6H_{10}O_4$	95-92-1	Esters	97
		1067-20-5		
3,3-Diethylpentane	C ₉ H ₂₀ .		q-Alkanes	84
Diethylperoxide	$C_4H_{10}O_2$	628-37-5	Peroxide	97
Diethyl phthalate	$C_{12}H_{14}O_4$	84-66-2	Esters	97
Diethyl o-phthalate	$C_{12}H_{14}O_4$	84-66-2	Esters	97
Diethyl 1,2-phthalate	$C_{12}H_{14}O_4$	84-66-2	Esters	97
Diethyl propanedioate	$C_7H_{12}O_4$	105–53–3	Esters	97-
Diethyl succinate	$C_8H_{14}O_4$	123-25-1	Esters	974,975
2,2-Diethylsuccinic acid	C ₈ H ₁₄ O ₄	5692-97-7	Acids	95
meso-2,3-Diethylsuccinic acid	$C_8H_{14}O_4$	35392-80-4	Acids	95
racemic-2,3-Diethylsuccinic acid	$C_8H_{14}O_4$	35392-77-9	Acids	954,95
2,2-Diethylsuccinic anhydride	C ₈ 11 ₁₂ O ₃	2840-69-9	Anhydrides	96.
Diethyl sulfate	$C_4H_{10}O_4S$	64-67-5	Sulfates	1055
Diethyl sulfide	$C_4H_{10}S$	352-93-2	Sulfides	1041,1042
Diethyl sulfite	$C_4H_{10}O_3S$	623-81-4	Sulfites	105
	C ₄ H ₁₀ O ₃ S C ₄ H ₁₀ O ₂ S	597353		
Diethyl sulfone			Sulfones	1051
Diethyl sulfoxide	$C_4H_{10}OS$	70-29-1	Sulfoxides	1049
Diethanoyl peroxide	$C_4H_6O_4$	110-22-5	Peroxide	978
N,N-Diethylurea	$C_5H_{12}N_2O$	634-95-7	Ureas	1012
1.2-Difluorobenzene	$C_6H_4F_2$	367-11-3	Fluoride	106
1,3-Difluorobenzene	$C_6H_4F_2$	372-18-9	Fluoride	1061
1,4-Difluorobenzene	$C_6H_4F_2$	540-36-3	Fluoride	1061
2,2'-Difluorobiphenyl	$C_{12}H_8F_2$	388-82-9	Fluoride	1061
4,4'-Difluorobiphenyl	$C_{12}H_8F_2$	398-23-2	Fluoride	1061,1062
1,1-Difluoroethane	$C_2H_4F_2$	75-37-6	Fluoride	1059
1,1-Difluoroethylene	$C_2H_2F_2$	75~38~7	Fluoride	1059,1060
1,2-Difluorotetrachloroethane	$C_2Cl_4F_2$	76-12-0	Mixed	1100
Di-n-hexyl disulfide	C ₁₂ H ₂₆ S ₂	10496-15-8	Disulfides	1049
	C ₁₂ H ₂₆ S	6294-31-1	Sulfides	1045,1046
Di-n-hexyl sulfide				•
Dihyrofuran-2,5-dione	C ₄ H ₄ O ₃	108-30-5	Anhydrides	964
2,3-Dihydrothiophene	C₄H ₆ S	1120–59–8	CyclCHS	1058
2,5-Dihydrothiophene	C₄H ₆ S	1708–32–3	CyclCHS	1058
2,3-Dihydroxynaphthalene	$C_{10}H_8O_2$	92-44-4	Alcohols	925
1,2-Diiodobenzene	$C_6H_4I_2$	615-42-9	Iodide	1096
1,3-Diiodobenzene	$C_6H_4I_2$	626-00-6	Iodide	1096
1,4-Diiodobenzene	$C_6H_4I_2$	624-38-4	Iodide	1090
1,2-Diiodobutane	$C_4H_8I_2$	53161-72-1	Iodide	1094
1,3-Diiodocyclobutane(cis/trans)	$C_4H_6I_2$	not available	Iodide	1090
1,3-Diiodocyclobutane (Z)	$C_4H_6I_2$	4934–57-0	Iodide	
1,3-Diiodocyclobutane (E)	$C_4H_6I_2$	4943–56–9	Iodide	
1.2-Diiodocyclobutane (E)	C ₂ H ₄ I ₂	624-73-7	Iodide	1093
-,		590-27-2	Iodide	1094
1,2-Diiodoethylene (E)	$C_2H_2I_2$			
1,2-Diiodoethylene (Z)	$C_2H_2I_2$	590-26-1	Iodide	1094
1,2-Diiodopropane	$C_3H_6I_2$	598-29-8	Iodide	109:
Diisobutylamine	$C_8H_{19}N$	110-96-3	Amines	980
Diisobutyl sulfide	$C_8H_{18}S$	592654	Sulfides	1044
Diisobutyl sulfone	$C_8H_{18}O_2S$	10495-45-1	Sulfones	1052
Diisopentyl sulfide	C ₁₀ H ₂₂ S	544-02-5	Sulfides	1044
Diisopropylamine	$C_6H_{15}N$	108-18-9	Amines	986
Disopropyldiazene	C ₆ H ₁₄ N ₂	3880-49-7	Diazene	99:
Disopropyl ether	C ₆ H ₁₄ O	108-20-3	Ethers	928
	C ₂ H ₁₄ O	565-80-0	Ketones	941
Diisopropyl ketone				
Diisopropyl sulfide	C ₆ H ₁₄ S	625-80-9	Sulfides	1043
	$C_8H_{10}O_2$	91-16-7	Ethers	934
1,2-Dimethoxybenzene 1,1-Dimethoxyethane	$C_4H_{10}O_2$	25154-53-4	Ethers	930

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
Dimethoxymethane	C ₃ H ₈ O ₂	109–87–5	Ethers	929
2,2-Dimethoxypropane	$C_5H_{12}O_2$	77–76–9	Ethers	930
N,N-Dimethylacetamide	C ₄ H ₉ NO	127-19-5	Amides	1010
Dimethylamine	C₂H ₇ N	124-40-3	Amines	985
N,N-Dimethylaniline	C ₈ H ₁₁ N	121–69–7 95–47–6	Amines	990
1,2-Dimethylbenzene	$C_8H_{10} \\ C_8H_{10}$	95-47-6 108-38-3	Aromat01 Aromat01	863
1,3-Dimethylbenzene 1,4-Dimethylbenzene	C ₈ H ₁₀	106-42-3	Aromat01	863
2,3-Dimethyl benzoic acid	C ₉ H ₁₀ O ₂	603-79-2	Acids	863,864 957
2,4-Dimethyl benzoic acid	C ₉ H ₁₀ O ₂	611–01–8	Acids	957,958
2,5-Dimethyl benzoic acid	C ₉ H ₁₀ O ₂	610-72-0	Acids	958
2,6-Dimethyl benzoic acid	$C_9H_{10}O_2$	632-46-2	Acids	958
3,4-Dimethyl benzoic acid	$C_9H_{10}O_2$	619-04-5	Acids	958
3,5-Dimethyl benzoic acid	$C_9H_{10}O_2$	499-06-9	Acids	958,959
trans-2,3-Dimethylbicyclo[2.2.1]heptane	C9H16	20558-16-1	Cyclic03	906
7,7-Dimethylbicyclo[2.2.1]heptane	C9H16	2034-53-9	Cyclic03	906
4,4'-Dimethylbiphenyl	$C_{14}H_{14}$	613-33-2	Aromat02	879
2,3-Dimethyl-1,3-butadiene	C_6H_{10}	513-81-5	s-Alkenes	858
2,2-Dimethylbutane	C_6H_{14}	75–83–2	q-Alkanes	842
2,3-Dimethylbutane	C ₆ H ₁₄	79–29–8	t-Alkanes	841
2,2-Dimethyl-1,4-butanedioic acid	$C_6H_{10}O_4$	597–43–3	Acids	954
meso-2,3-Dimethyl-1,4-butanedioic acid	$C_6H_{10}O_4$	608-40-2	Acids	954
racemic-2,3-Dimethyl-1,4-butanedioic acid	$C_6H_{10}O_4$	608–39–9	Acids	954,955
2,3-Dimethyl-2-butanethiol	C ₆ H ₁₄ S	1639016	Thiols	1040
3,3-Dimethyl-2-butanone	C ₆ H ₁₂ O	75-97-8	Ketones	941
2,3-Dimethyl-1-butene 2,3-Dimethyl-2-butene	C ₆ H ₁₂	563-78-0	s-Alkenes	855
3,3-Dimethyl-1-butene	C_6H_{12} C_6H_{12}	563-79-1 558-37-2	s-Alkenes s-Alkenes	855
Dimethyl (Z)-2-butenedioate	C ₆ H ₈ O ₄	624-48-6	Esters	856
3,3-Dimethyl-1-butyne	C ₆ H ₁₀	693-02-7	Alkynes	974 862
1,1-Dimethylcyclohexane	C ₈ H ₁₆	590-66-9	Cyclic02	897
trans-1,2-Dimethylcyclohexane	C ₈ H ₁₆	6876–23–9	Cyclic02	897
trans-1,3-Dimethylcyclohexane	C_8H_{16}	2207036	Cyclic02	897
trans-1,4-Dimethylcyclohexane	C_8H_{16}	2207-04-7	Cyclic02	897
1,1-Dimethylcyclopentane	C7H14	1638-26-2	Cyclic01	892
cis-1,2-Dimethylcyclopentane	C_7H_{14}	1192–18–3	Cyclic01	892
trans-1,2-Dimethylcyclopentane	C_7H_{14}	822-50-4	Cyclic01	892
trans-1,3-Dimethylcyclopentane	C7H14	1759–58–6	Cyclic01	892
Dimethyldiazene	$C_2H_6N_2$	503-28-6	Diazene	998
2,5-Dimethyldiphenylmethane	$C_{15}H_{16}$	13540-50-6	Aromat02	875
N,N'-Dimethyl-N,N'-diphenylurea	$C_{15}H_{16}N_2O$	611-92-7	Ureas	1013
Dimethyl disulfide	C ₂ H ₆ S ₂	624-92-0	Disulfides	1048
N,N-Dimethylethanamide	C₄H ₉ NO	127-19-5	Amides	1010
Dimethyl ethanedioate Dimethyl ether	C₄H ₆ O₄ C₂H ₆ O	553-90-2	Esters	974
N,N-Dimethylformamide	C₃H₁NO	115-10-6 68-12-2	Ethers	926
2,6-Dimethyl-4-heptanone	C ₉ H ₁₈ O	108-83-8	Amides Ketones	1008
2,2-Dimethylhexane	C_8H_{18}	590-73-8	q-Alkanes	942 843
2,3-Dimethylhexane	C ₈ H ₁₈	584–94–1	t-Alkanes	841
2,4-Dimethylhexane	C ₈ H ₁₈	589–43–5	t-Alkanes	840
2,5-Dimethylhexane	C ₈ H ₁₈	592-13-2	t-Alkanes	840
3,3-Dimethylhexane	C ₈ H ₁₈	563-16-6	q-Alkanes	843
3,4-Dimethylhexane	C_8H_{18}	583-48-2	t-Alkanes	841
cis-2,2-Dimethyl-3-hexene	C_8H_{16}	690926	s-Alkenes	854,855
trans-2,2-Dimethyl-3-hexene	C_8H_{16}	690-93-7	s-Alkenes	855
cis-2,5-Dimethyl-3-hexene	C_8H_{16}	10557-44-5	s-Alkenes	856
trans-2,5-Dimethyl-3-hexene	C_8H_{16}	692-70-6	s-Alkenes	857
1,1-Dimethylhydrazine	$C_2H_8N_2$	57-14-7	Hydrazines	997
1,2-Dimethylhydrazine	$C_2H_8N_2$	540-73-8	Hydrazines	998
Dimethyl isophthalate	$C_{10}H_{10}O_4$	1459–93–4	Esters	976,977
Dimethyl ketone	C ₃ H ₆ O	67-64-1	Ketones	938
Dimethyl maleate	$C_6H_8O_4$	624-48-6	Esters	974
N,N-Dimethylmethanamide	C ₃ H ₇ NO	68–12–2	Amides	1008
1,2-Dimethylnaphthalene	$C_{12}H_{12}$	573-98-8	Aromat02	881
1,3-Dimethylnaphthalene	C ₁₂ H ₁₂	575-41-7	Aromat02	882
1,4-Dimethylnaphthalene	$C_{12}H_{12}$	571584	Aromat02	882

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
1,5-Dimethylnaphthalene	C ₁₂ H ₁₂	571-61-9	Aromat02	882
1,6-Dimethylnaphthalene	$C_{12}H_{12}$	575-43-9	Aromat02	882
1,7-Dimethylnaphthalene	$C_{12}H_{12}$	575–37–1	Aromat02	882
1,8-Dimethylnaphthalene	$C_{12}H_{12}$	569-41-5	Aromat02	883
2,3-Dimethylnaphthalene	$C_{12}H_{12}$	581-40-8	Aromat02	883
2,6-Dimethylnaphthalene	$C_{12}H_{12}$	581-42-0	Aromat02	883
2,7-Dimethylnaphthalene	$C_{12}H_{12}$	582-16-1	Aromat02	883
Dimethylnitramine	C ₂ H ₆ N ₂ O ₂	4164287	Nitramines	1033
Dimethylnitrosoamine	$C_2H_6N_2O$	62-75-9	Nitroso	1021
2,7-Dimethyloctane	$C_{10}H_{22}$	1072–16–8	t-Alkanes	842
Dimethyl oxalate	C ₄ H ₆ O ₄	553-90-2	Esters	974
3,3-Dimethylpenta-1,4-diyne	C_7H_8	62496-43-9	Alkynes	862
2,2-Dimethylpentane	C ₇ H ₁₆	590-35-2	q-Alkanes	
•	C ₇ H ₁₆ C ₇ H ₁₆	565-59-3	-	842,843
2,3-Dimethylpentane			t-Alkanes	841
2,4-Dimethylpentane	C ₇ H ₁₆	108-08-7	t-Alkancs	840
3,3-Dimethylpentane	C ₇ H ₁₆	562–49–2	q-Alkanes	843
2,2-Dimethyl-3-pentanone	$C_7H_{14}O$	564-04-5	Ketones	941
2,4-Dimethyl-3-pentanone	$C_7H_{14}O$	565-80-0	Ketones	941
2,4-Dimethyl-1-pentene	C_7H_{14}	2213-32-3	s-Alkenes	855
2,4-Dimethyl-2-pentene	C_7H_{14}	625-65-0	s-Alkenes	855
cis-4,4-Dimethyl-2-pentene	C_7H_{14}	762-63-0	s-Alkenes	856
trans-4,4-Dimethyl-2-pentene	C ₇ H ₁₄	690-08-4	s-Alkenes	856
Dimethylperoxide	C ₂ H ₆ O ₂	690–028	Peroxide	978
2,3-Dimethylphenol	C ₈ H ₁₀ O	526-75-0	Alcohols	922
2,4-Dimethylphenol	C8H10O	105-67-9	Alcohols	922
•		95–87–4		
2,5-Dimethylphenol	C ₈ H ₁₀ O		Alcohols	923
2,6-Dimethylphenol	C ₈ H ₁₀ O	576–26–1	Alcohols	923
3,4-Dimethylphenol	$C_8H_{10}O$	95–65–8	Alcohols	923
3,5-Dimethylphenol	$C_8H_{10}O$	108–68–9	Alcohols	923
Dimethyl phthalate	$C_{10}H_{10}O_4$	131–11–3	Esters	976
Dimethyl m-phthalate	$C_{10}H_{10}O_4$	1459–93–4	Esters	976,977
Dimethyl o-phthalate	$C_{10}H_{10}O_4$	131-11-3	Esters	976
Dimethyl p-phthalate	$C_{10}H_{10}O_4$	120-61-6	Esters	977
Dimethyl 1,2-phthalate	$C_{10}H_{10}O_4$	131-11-3	Esters	976
Dimethyl 1,3-phthalate	$C_{10}H_{10}O_4$	1459-93-4	Esters	976,977
Dimethyl 1,4-phthalate	$C_{10}H_{10}O_4$	120-61-6	Esters	977
2,2-Dimethylpropanamide	C ₅ H ₁₁ NO	754–10–9	Amides	1007
N,N-Dimethylpropanamide	C ₅ H ₁₁ NO	758-96-3	Amides	1007
2,2-Dimethylpropane	C₅H ₁₂	463-82-1	q-Alkanes	842
2,2-Dimethylpropane-1,3-dinitrile	C ₅ H ₆ N ₂	7321–55–3	Nitriles	996
2,2-Dimethyl-1-propanethiol	C ₅ H ₁₂ S	1679–08–9	Thiols	1040
2,2-Dimethylpropanenitrile	C₅H ₉ N	630-18+2	Nitriles	995
2,2-Dimethylpropanoic acid	$C_5H_{10}O_2$	75-98-9	Acids	950
2,2-Dimethylpropanoic anhydride	$C_{10}H_{18}O_3$	1538-75-6	Anhydrides	964
N,N-Dimethylpropionamide	C ₅ H ₁₁ NO	758–96–3	Amides	1009
2.2-Dimethylpropyl ethanoate	$C_6H_{12}O_2$	540-88-5	Esters	970
2,3-Dimethylpyridine	C ₇ H ₉ N	583-61-9	CyclCHN	1004
2,4-Dimethylpyridine	C ₇ H ₉ N	108-47-4	CyclCHN	1005
2,5-Dimethylpyridine	C ₇ H ₉ N	589–93–5	CyclCHN	1005
2,6-Dimethylpyridine	C7H9N	108-48-5	CyclCHN	1005
			CyclCHN	
3,4-Dimethylpyridine	C ₇ H ₉ N	583–58–4	•	1005
3,5-Dimethylpyridine	C ₇ H ₉ N	591-22-0	CyclCHN	1005
2,5-Dimethylpyrrole	C ₆ H ₉ N	625-84-3	CyclCHN	1002
(cis-3,7a-H)-(cis-5,7a-H)-3,5-Dimethyl-pyrrolizidine	$C_9H_{17}N$	56160-71-5	CyclCHN	1006
2,2-Dimethylsuccinic acid	$C_6H_{10}O_4$	597-43-3	Acids	954
2,2-Dimethylsuccinic anhydride	$C_6H_8O_3$	17347614	Anhydrides	964,965
meso-2,3-Dimethylsuccinic acid	$C_6H_{10}O_4$	608-40-2	Acids	954
racemic-2,3-Dimethylsuccinic acid	C ₆ H ₁₀ O ₄	608-39-9	Acids	954,955
Dimethyl sulfate	C ₂ H ₆ O ₄ S	77–78–1	Sulfates	1055
Dimethyl sulfide	C ₂ H ₆ S	75–18–3	Sulfides	1033
•				1055
Dimethyl sulfite	C ₂ H ₆ O ₃ S	616-42-2	Sulfites	
Dimethyl sulfone	C ₂ H ₆ O ₂ S	67-71-0	Sulfones	1050
Dimethyl sulfoxide	C₂H ₆ OS	67–68–5	Sulfoxides	1049
Dimethyl terephthalate	$C_{10}H_{10}O_4$	120–61–6	Esters	977
N,N-Dimethylurea	$C_3H_8N_2O$	598-94-7	Ureas	1011

TABLE 56. Name and Formula Index - Continued

2.4-Distrocasiline	Name	Formula	CAS Registry No.	Family	Page
2.5 Dintroaniline	2,3-Dinitroaniline				1029
2.45 Distributionalities	,				1029
3.4 Dinitronalline	· ·				1029
33-Dinitronathine	· ·				1030
1.2.Dinitrobenzene	•				1030
1.3-Dinitrobenzene	•				1030
1.4-Dinitrobenzene					1025
JDinitrobutane	- -				1025
1.1-Dinitrochane	· ·				1025
1.2-Dinitroentame					1024,1025
Districtor CH ₃ N ₂ O ₂ 625-76-3 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 51-28-5 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 51-28-5 Nitros 10 1,1-Districtorphenol C,H ₄ N ₂ O ₂ 51-28-5 Nitros 10 1,1-Districtorphenol C,H ₄ N ₂ O ₂ 6125-21-9 Nitros 10 1,1-Districtorphenol C,H ₄ N ₂ O ₂ 6125-21-9 Nitros 10 1,1-Districtorphenol C,H ₄ N ₂ O ₂ 6125-21-9 Nitros 10 1,1-Districtorphenol C,H ₄ N ₂ O ₂ 595-49-3 Nitros 10 2,2-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 3,7-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 3,7-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 3,7-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 101-25-7 Nitros 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 102-25-6 Ethers 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 102-25-6 Ethers 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 102-20-2 Ethers 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 102-20-2 Ethers 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 102-20-1 Ethers 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 102-20-1 Ethers 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 102-20-1 Ethers 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂ 102-20-1 Ethers 10 2,4-Districtorphenol C,H ₄ N ₂ O ₂	•				1024
1.1-Dinitropentane	•				1024
2.4-Disitrophenol					1022
2.6-Dinitrophenol	•				1024
1.1-Dinitropropane	•				1028
1.3-Dinitropropane					1028
2,2-Dinitropropane C,H _A N _O ; 95-49-3 Nitros 10 3,7-Dinitrosopatamethylenetetramine C,H _A N _O ; 101-25-7 Nitros 10 3,7-Dinitrosopatamethylenetetramine C,H _A N _O ; 101-25-7 Nitros 10 2,4-Dinitrotoluene C,H _A N _O ; 101-25-7 Nitros 10 2,5-Dinitrotoluene C,H _A N _O ; 101-25-7 Nitros 10 3,5-Dioxaleprane C,H _A O; 402-25-3 Ethers 10 3,5-Dioxaleprane C,H _A O; 123-91-1 Ethers 9 1,4-Dioxane C,H _A O; 123-91-1 Ethers 9 1,4-Dioxane C,H _A O; 305-65-7 Ethers 9 1,3-Dioxolane C,H _A O; 466-06-0 Ethers 9 1,3-Dioxolane-2-one C,H _A O; 404-06-0 Ethers 9 Di-n-pentyl sulfide C,H _A D; 927-49-1 Ketones 9 Di-n-pentyl sulfide C,H _A D; 327-10-6 Sulfides 10 Di-n-pentyl sulfide <t< td=""><td>• •</td><td></td><td></td><td></td><td>1024</td></t<>	• •				1024
1,5-Dintrosopentamethylenetetramine C,H ₀ N ₀ C ₂ 101-25-7 Nitroso 10 2,4-Dintrotoluene C,H ₀ N ₀ C ₃ 101-25-7 Nitroso 10 2,4-Dintrotoluene C,H ₀ N ₀ C ₄ 121-14-2 Nitros 10 2,4-Dintrotoluene C,H ₀ N ₀ C ₄ 121-14-2 Nitros 10 10 125-10 10 10 10 10 10 10 10					1024
3,7-Dinitroso-1,3,5,7-tetraza-bicyclo[3,3,1]nonane					1025
2.4 Dinitrotoluene ChLN-O ₄ 121-14-2 Nitros 10 2.6 Dinitrotoluene ChLN-O ₄ 66-20-2 Nitros 10 3.5 Dioxaheptane ChLi-O ₂ 462-95-3 Ethers 9 1.3 Dioxane ChLi-O ₂ 505-22-6 Ethers 9 1.3 Dioxane ChLi-O ₂ 505-65-7 Ethers 9 1.3 Dioxolane ChLi-O ₂ 606-06-0 Ethers 9 1.3 Dioxolan-2-one ChLO ₃ 96-49-1 Carbonates 9 1.3 Dioxolan-2-one ChLO ₃ 96-49-1 Carbonates 9 1.3 Dioxolan-2-one ChLO ₃ 96-49-1 Carbonates 9 1.3 Dioxolan-2-one ChLO ₃ 927-49-1 Ketones 9 1.3 Dioxolan-2-one ChLO ₄ 927-49-1 Ketones 9 1.3 Dioxolan-2-one ChLI-O ₄ 927-49-1 Ketones 9 1.3 Dioxolan-2-one ChLI-O ₄ 927-49-1 Ketones 9 1.4 Diphenylethenylethene ChLI-O ₄ 927-49					1022
2,6-Dinitrotoluene					1022
3.5-Dickaseptane	•				1027
1,3-Dioxane C,H _O 2 505-22-6 Ethers 9 1,3-Dioxane C,H _O 2 123-91-1 Ethers 9 1,3-Dioxosane C,H _O 2 505-65-7 Ethers 9 1,3-Dioxosane C,H _O 2 646-06-0 Ethers 9 1,3-Dioxosane-2-one G,H _O 2 646-06-0 Ethers 9 3,3-Dioxosane-2-one C,H _O 2 967-49-1 Carbonates 9 18-n-pentyl kletone C ₁ H ₂ O 927-49-1 Ketones 9 18-n-pentyl kletone C ₁ H ₂ O 927-49-1 Ketones 9 18-n-pentyl kletone C ₁ H ₁ O 951-65-5 Aromatic 10 Diphenylacetylene C ₁ H ₁ O 123-13-4 Acids 9 18-n-pentyl kletone C ₁ H ₁ O 1225-13-4 Acids 9 18-n-pentyl kletone C ₁ H ₁ O 1225-13-4 Acids 9 18-n-pentyl kletone C ₁ H ₁ O 1229-0 Cardonates 9 19-phenylethanedidio acid C ₁ H ₁ O 192-9-0<	•				1027
1,4-Dioxepane 1,3-Dioxepane 1	•				930
1,3-Dioxopane 1,3-Dioxolane	*				933
1,3-Dioxolane C3H ₄ O ₂ 64-00-0 Ethers 9 Ji-3-Dioxolan-2-one C3H ₄ O ₅ 96-49-1 Carbonates 9 Ji-π-pentyl disulfide C1H ₂ O ₅ 112-51-6 Disulfides 10 Di-π-pentyl sulfide C1H ₂ O ₅ 27-49-1 Ketones 9 Di-n-pentyl sulfide C1H ₁₀ O 927-49-1 Ketones 9 Di-n-pentyl sulfide C1H ₁₀ O 927-49-1 Ketones 9 Diphenylacetylene C4H ₁₀ O 91-5-5 Aromat02 8 meso-2,3-Diphenylbutanedioic acid C1H ₁ O ₄ 1225-13-4 Acids 9 meso-2,3-Diphenylbutanedioic acid C1 ₁ H ₁₀ O ₄ 41915-64-4 Acids 9 piphenyl-cylopropane C1 ₂ H ₁₀ O ₄ 1138-43-3 Cyclic03 9 vis-Diphenylbeyclopropane C1 ₂ H ₁₀ O ₄ 1138-47-2 Cyclic03 9 Diphenyl disulfide C1 ₂ H ₁₀ O ₂ 134-81-6 Ketones 9 Diphenyl disulfide C1 ₂ H ₁₀ O ₂ 104-9-0 Sulfides 10	•				934
1,3-Dioxolan-2-one C ₁ H ₄ O ₃ 96-49-1 Carbonates 99 Di -n -pentyl disulfide C ₁₀ H ₂ S ₂ 112-51-6 Disulfides 100 Di -n -pentyl sulfide C ₁₀ H ₂ S ₂ 112-51-6 Disulfides 100 Di -n -pentyl sulfide C ₁₀ H ₂ S ₃ 872-10-6 Sulfides 100 Diphenylacetylene C ₁₄ H ₁₀ 501-65-5 Aromat02 88 aras, Janus 1,4-Diphenyl-1,3-butadiene C ₁₆ H ₁₄ 538-81-8 Cyclic03 99 aras, Janus 1,4-Diphenyl-1,3-butadiene C ₁₆ H ₁₄ 538-81-8 Cyclic03 99 arasemic-2,3-Diphenylbutanedioic acid C ₁₆ H ₁₄ O ₄ 41915-64-4 Acids 99 order of the color of t					934 933
Di-n-pentyl disulfide CnHs2S2 112-51-6 Disulfides 10 Di-n-pentyl ketone CnHs2O 927-49-1 Ketones 9 Di-n-pentyl sulfide CnHs2S 872-10-6 Sulfides 10 Diphenylacetylene CnHs1 501-65-5 Aromat02 8 trass pans -1,4-Diphenyl-1,3-butadiene CnHs1 501-65-5 Aromat02 8 meso-2,3-Diphenylbutanedioic acid CnHs1-04 1225-13-4 Acids 9 meso-2,3-Diphenylbutanedioic acid CnHs1-04 41915-64-4 Acids 9 Diphenyl carbonate CnHs1-04 41915-64-4 Acids 9 cis-Diphenylbeyclopropane CnHs1-4 1138-48-3 Cyclic03 9 trass-Diphenylbeyclopropane CnHs1-4 1138-48-3 Cyclic03 9 Diphenyl disetone CnHs1-4 1138-48-3 Cyclic03 9 Diphenyl disetone CnHs1-4 1138-48-3 Cyclic03 9 Diphenyl disetone CnHs1-6 Ketones 9 Diphenylbudais	· ·				982
Di-n-pentyl ketone C ₁ H ₂ O 927-49-1 Ketones 9 Di-n-pentyl sulfide C ₁₀ H ₂₈ S 872-10-6 Sulfides 10 Di-n-pentyl sulfide C ₁₀ H ₁₀ 501-65-5 Aromat02 8° brans Janus - 1,4-Diphenyl-1,3-butadiene C ₁₀ H ₁₀ 538-81-8 Cyclic03 9 meso-2,3-Diphenylbutandedioic acid C ₁₀ H ₁₀ O 1225-13-4 Acids 9 Diphenyl carbonate C ₁₀ H ₁₀ O 192-09-0 Carbonates 9 6z-Diphenylcyclopropane C ₁₅ H ₁₄ 1138-48-3 Cyclic03 9 biphenyl disculfore C ₁₅ H ₁₀ 134-81-6 Ketones 9 Diphenyl disulfide C ₁₂ H ₁₀ S ₂ 82-33-7 Disulfides 10 Diphenyl disulfone C ₁₂ H ₁₀ O ₈ S ₂ 10409-06-0 Sulfones 10 1,1-Diphenylcylodecane C ₂ H ₁₀ O ₈ S ₂ 10409-06-0 Sulfones 10 1,1-Diphenylethane C ₁₄ H ₁₄ 612-00-0 Aromat02 8 1,1-Diphenylethane C ₁₄ H ₁₄ 103-29-7 Aro					1048
Di-π-penyl sulfide C ₁₀ H ₃ S 872-10-6 Sulfides 10 Diphenylacetylene C ₁₄ H ₁₀ 501-65-5 Aromat02 8 trans trans 1,4-Diphenyl-1,3-butadiene C ₁₆ H ₁₀ A 1225-13-4 Acids 9 meso-2,3-Diphenylbutanedioic acid C ₁₆ H ₁₀ O ₄ 41915-64-4 Acids 9 racemic-2,3-Diphenylbutanedioic acid C ₁₈ H ₁₀ O ₃ 102-09-0 Carbonates 9 cis-Diphenyl carbonate C ₁₈ H ₁₄ 1138-48-3 Cyclic03 9 cis-Diphenyl carbonate C ₁₈ H ₁₄ 1138-48-3 Cyclic03 9 cis-Diphenylcyclopropane C ₁₈ H ₁₄ 1138-47-2 Cyclic03 9 Diphenyl dikteune C ₁₄ H ₁₀ O ₂ 134-81-6 Ketones 9 Diphenyl distuffore C ₁₂ H ₁₀ O ₈ S ₂ 10409-06-0 Sulfones 10 Diphenyl distuffore C ₁₂ H ₁₀ O ₈ S ₂ 10409-06-0 Sulfones 10 1,1-Diphenylethane C ₁₄ H ₁₄ 612-00-0 Aromat02 8 1,1-Diphenylethane C ₁₄ H ₁₄ 612-0					940
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	- ·				1045
wans, rams-1, d-Diphenyl-1,3-butadiene C ₁₆ H ₁₄ O ₄ 1225-13-4 Acids 90 meso-2,3-Diphenylbutanedioic acid C ₁₆ H ₁₄ O ₄ 1225-13-4 Acids 90 acemic-2,3-Diphenylbutandedioic acid C ₁₆ H ₁₄ O ₄ 41915-64-4 Acids 90 Diphenyl carbonate C ₁₅ H ₁₄ 1138-48-3 Cyclic03 90 biphenylcyclopropane C ₁₅ H ₁₄ 1138-47-2 Cyclic03 90 Diphenyl disulfide C ₁₆ H ₁₆ O ₂ 134-81-6 Ketones 99 Diphenyl disulfide C ₁₂ H ₁₆ O ₂ 882-33-7 Disulfides 10 Diphenyl disulfone C ₁₂ H ₁₆ O ₂ S ₂ 882-33-7 Disulfides 10 1,1-Diphenylethane C ₁₄ H ₁₄ 610-0-0 Aromat02 88 1,2-Diphenylethane C ₁₄ H ₁₄ 103-29-7 Aromat02 88 1,2-Diphenylethane C ₁₄ H ₁₄ 103-29-7 Aromat02 88 1,2-Diphenylethane C ₁₄ H ₁₀ O ₂ 134-81-6 Ketones 99 Diphenylethane C ₁₄ H ₁₀ O ₂ 134-81-6 <td>- · ·</td> <td></td> <td></td> <td></td> <td>877</td>	- · ·				877
meso-2,3-Diphemylbutanedioic acid $C_{10}H_{14}O_4$ $1225-13-4$ Acids 90 racemic-2,3-Diphenylbutanedeioic acid $C_{11}H_{14}O_4$ $41915-64-4$ Acids 90 piphenyl carbonate $C_{11}H_{14}O_3$ $102-09-0$ Carbonates 90 cis-Diphenylcyclopropane $C_{11}H_{14}$ $1138-48-3$ Cyclic03 90 piphenyl diketone $C_{11}H_{10}O_2$ $134-81-6$ Ketones 99 Diphenyl disulfide $C_{12}H_{10}O_2$ $882-33-7$ Disulfides 10 Diphenyl disulfone $C_{12}H_{10}O_2$ $10409-06-0$ Sulfones 10 $1,1-Diphenyl dodecane C_{21}H_{10}O_3 10409-06-0 Sulfones 10 1,1-Diphenyl dodecane C_{21}H_{10}O_3 10409-06-0 Aromat02 88 1,1-Diphenyl dodecane C_{21}H_{10}O_3 10409-06-0 Aromat02 88 1,1-Diphenyl dodecane C_{11}H_{11} 612-00-0 Aromat02 88 1,1-Diphenyl dodecane C_{11}H_{10}O_3 134-81-6 Ketones 90 $					908
racemic-2,3-Diphenylbutandedioic acid $C_{18}H_{10}O_3$ $102-09-0$ Carbonates 90 $C_{18}H_{10}O_3$ $102-09-0$ Carbonates 90 $C_{18}Dliphenylcyclopropane C_{18}H_{14} 1138-48-3 Cyclic03 90 C_{18}Dliphenylcyclopropane C_{18}H_{10}O_2 134-81-0 Ketones 90 Diphenyl disulfide C_{18}H_{10}O_2 134-81-0 Ketones 90 Diphenyl disulfide C_{18}H_{10}O_2 1049-06-0 Sulfones 100 Diphenyl disulfide C_{18}H_{10}O_4S_2 10409-06-0 Sulfones 100 1,1-Diphenyldedecane C_{28}H_{34} 1603-53-8 Aromat02 88 1,1-Diphenylethane C_{18}H_{10} 103-29-7 Aromat02 88 1,2-Diphenylethane C_{18}H_{10} 134-81-6 Ketones 90 Diphenylethane C_{18}H_{10} 134-81-6 Ketones 90 Diphenylethane C_{18}H_{10} 134-81-6 Ketones 90 Diphenylethane C$					963
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cts -Diphenylcyclopropane $C_{15}H_{14}$ $1138-48-3$ Cyclic03 90 trans -Diphenylcyclopropane $C_{15}H_{14}$ $1138-47-2$ Cyclic03 90 piphenyl disulfide $C_{12}H_{10}O_2$ $18-41-6$ Ketones 90 Diphenyl disulfide $C_{12}H_{10}O_3$ $882-33-7$ Disulfides 10 Diphenyl disulfide $C_{12}H_{10}O_3$ $10409-06-0$ Sulfones 10 Diphenyl disulfide $C_{12}H_{10}O_3$ $10409-06-0$ Sulfones 10 1,1-Diphenyldodecane $C_{14}H_{14}$ $1603-53-8$ Aromat02 8 1,2-Diphenylethane $C_{14}H_{14}$ $103-29-7$ Aromat02 8 1,2-Diphenylethane $C_{14}H_{14}$ $103-29-7$ Aromat02 8 Diphenylether $C_{14}H_{10}O_2$ $134-81-6$ Ketones 9 1,1-Diphenylethyler $C_{14}H_{12}$ $530-48-3$ Aromat02 8 1,2-Diphenylhydrazine $C_{12}H_{10}O$ $101-84-8$ Ethers 9 1,2-Diphenylhydrazine C					982
trans-Diphenylcyclopropane $C_{13}H_{14}$ $1138-47-2$ $Cyclic03$ 90 Diphenyl diketone $C_{14}H_{10}O_2$ $134-81-6$ Ketones 99 Diphenyl disulfide $C_{12}H_{10}O_3$ $10409-06-0$ Disulfides 10 Diphenyl disulfone $C_{12}H_{10}O_4S_2$ $10409-06-0$ Sulfones 10 1,1-Diphenyledodecane $C_{24}H_{34}$ $1603-53-8$ Aromat02 88 1,2-Diphenylethane $C_{14}H_{14}$ $612-00-0$ Aromat02 88 1,2-Diphenylethane $C_{14}H_{14}$ $612-00-0$ Aromat02 88 1,2-Diphenylethane $C_{14}H_{14}$ $612-00-0$ Aromat02 88 Diphenyl ether $C_{14}H_{10}O_2$ $134-81-6$ Ketones 99 Diphenyl ether $C_{12}H_{10}O$ $101-84-8$ Ethers 90 1,2-Diphenylethylene $C_{14}H_{12}$ $530-48-3$ Aromat02 $875,873$ 1,2-Diphenylethylene $C_{13}H_{10}O$ $119-61-9$ Ketones 99 Diphenyl exidone $C_{13}H_{10}O$ <td></td> <td></td> <td></td> <td></td> <td>908</td>					908
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	• • • •			•	908
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$					945
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Diphenyl disulfide	$C_{12}H_{10}S_2$	882-33-7	Disulfides	1049
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Diphenyl disulfone	$C_{12}H_{10}O_4S_2$	10409060	Sulfones	1054
1,1-Diphenylethane $C_{14}H_{14}$ $612-00-0$ Aromat02 87 1,2-Diphenylethane $C_{14}H_{14}$ $103-29-7$ Aromat02 87 Diphenylethanedione $C_{14}H_{10}O_2$ $134-81-6$ Ketones 94 Diphenyl ether $C_{12}H_{10}O$ $101-84-8$ Ethers 95 1,1-Diphenylethylene $C_{14}H_{12}$ $530-48-3$ Aromat02 875,83 1,2-Diphenylhydrazine $C_{12}H_{12}N_2$ $122-66-7$ Hydrazines 95 1,2-Diphenylhydrazine $C_{13}H_{10}O$ $119-61-9$ Ketones 94 Diphenyl ketone $C_{13}H_{10}O$ $119-61-9$ Ketones 94 Diphenyl suifore $C_{13}H_{10}O$ $101-81-8$ Ethers 93 Jabersylvatione $C_{12}H_{10}O$ $101-81-8$	1,1-Diphenyldodecane	$C_{24}H_{34}$	1603-53-8		875
1,2-Diphenylethane $C_{14}H_{14}$ 103-29-7 Aromat02 87 Diphenylethanedione $C_{14}H_{10}O_2$ 134-81-6 Ketones 96 Diphenyl ether $C_{12}H_{10}O$ 101-84-8 Ethers 92 1,1-Diphenylethylene $C_{14}H_{12}$ 530-48-3 Aromat02 875,87 1,2-Diphenylhydrazine $C_{12}H_{12}N_2$ 122-66-7 Hydrazines 96 Diphenyl ketone $C_{13}H_{10}O$ 119-61-9 Ketones 94 Diphenyl ketone $C_{13}H_{10}O$ 119-61-9 Ketones 94 Diphenyl ketone $C_{13}H_{10}O$ 101-81-5 Aromat02 87 Diphenyl ketone $C_{13}H_{10}O$ 101-84-8 Ethers 93 Diphenyl sulf $C_{12}H_{10}O$ 101-84-8 Ethers 93 Diphenyl-1,3-propanedione $C_{13}H_{12}O$ 120-46-7 Ketones 94 meso-2,3-Diphenylsuccinic acid $C_{14}H_{14}O$ 1225-13-4 Acids 96 racemic-2,3-Diphenylsuccinic acid $C_{14}H_{14}O$ 7584-72-7 Acids 96 Diphenyl sulffoxe $C_{12}H_{10}O$ S </td <td>1,1-Diphenylethane</td> <td></td> <td>612000</td> <td></td> <td>875</td>	1,1-Diphenylethane		612000		875
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1,2-Diphenylethane	$C_{14}H_{14}$	103-29-7	Aromat02	876
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Diphenylethanedione	$C_{14}H_{10}O_2$	134-81-6	Ketones	945
1,1-Diphenylethylene $C_{14}H_{12}$ 530-48-3 Aromat02 875,87 1,2-Diphenylhydrazine $C_{12}H_{12}N_2$ 122-66-7 Hydrazines 99 Diphenyl ketone $C_{13}H_{10}O$ 119-61-9 Ketones 94 Diphenyl ketone $C_{13}H_{12}$ 101-81-5 Aromat02 87 Diphenyl oxide $C_{12}H_{10}O$ 101-84-8 Ethers 93 1,3-Diphenyl-1,3-propanedione $C_{15}H_{12}O_2$ 120-46-7 Ketones 94 meso-2,3-Diphenylsuccinic acid $C_{15}H_{14}O_4$ 1225-13-4 Acids 96 racemic-2,3-Diphenylsuccinic acid $C_{16}H_{14}O_4$ 7584-72-7 Acids 96 Diphenyl sulfide $C_{12}H_{10}O_5$ 139-66-2 Sulfides 104 Diphenyl sulfone $C_{12}H_{10}O_5$ 127-63-9 Sulfones 105 Diphenylurea $C_{12}H_{10}O_5$ 945-51-7 Sulfoxides 105 N,N'-Diphenylurea $C_{13}H_{12}N_{2}O$ 603-54-3 Ureas 101 Dipropanoyl peroxide $C_{6}H_{10}O_4$ 3248-28-0 Peroxide 97 Dipropionyl peroxide	Diphenyl ether	$C_{12}H_{10}O$	101-84-8	Ethers	935
1,2-Diphenylhydrazine $C_{12}H_{12}N_2$ 122 -66-7 Hydrazines 99 Diphenyl ketone $C_{13}H_{10}O$ 119 -61-9 Ketones 94 Diphenylmethane $C_{13}H_{12}$ 101 -81-5 Aromat02 87 Diphenyl oxide $C_{12}H_{10}O$ 101 -84-8 Ethers 93 1,3-Diphenyl-1,3-propanedione $C_{15}H_{12}O_2$ 120 -46-7 Ketones 94 neso-2,3-Diphenylsuccinic acid $C_{16}H_{14}O_4$ 1225 -13-4 Acids 96 racemic-2,3-Diphenylsuccinic acid $C_{16}H_{14}O_4$ 7584 -72-7 Acids 96 Diphenyl sulfide $C_{12}H_{10}O_5$ 139 -66-2 Sulfides 104 Diphenyl sulfone $C_{12}H_{10}O_5$ 127 -63-9 Sulfones 105 Diphenyl sulfoxide $C_{12}H_{10}O_5$ 945 -51-7 Sulfoxides 105 N,N-Diphenylurea $C_{13}H_{12}N_{2}O$ 603 -54-3 Ureas 101 N,N'-Diphenylurea $C_{13}H_{12}N_{2}O$ 102 -07-8 Ureas 101 Dipropanoyl peroxide $C_{6}H_{10}O_4$ 3248 -28-0 Peroxide 97	1,1-Diphenylethylene	$C_{14}H_{12}$	530-48-3	Aromat02	875,876
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1,2-Diphenylhydrazine	$C_{12}H_{12}N_2$	122-66-7	Hydrazines	998
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Diphenyl ketone	$C_{13}H_{10}O$	119-61-9	Ketones	944
1,3-Diphenyl-1,3-propanedione $C_{15}H_{12}O_2$ $120-46-7$ Ketones 96 meso-2,3-Diphenylsuccinic acid $C_{16}H_{14}O_4$ $1225-13-4$ Acids 96 racemic-2,3-Diphenylsuccinic acid $C_{16}H_{14}O_4$ $7584-72-7$ Acids 96 Diphenyl sulfide $C_{12}H_{10}S$ $139-66-2$ Sulfides 104 Diphenyl sulfone $C_{12}H_{10}O_2S$ $127-63-9$ Sulfones 105 Diphenyl sulfoxide $C_{12}H_{10}OS$ $945-51-7$ Sulfoxides 105 N,N-Diphenylurea $C_{12}H_{10}OS$ $945-51-7$ Sulfoxides 105 N,N-Diphenylurea $C_{13}H_{12}N_{2}O$ $603-54-3$ Ureas 101 Dipropanoyl peroxide $C_{13}H_{12}N_{2}O$ $102-07-8$ Ureas 101 Dipropionyl peroxide $C_{6}H_{10}O_4$ $3248-28-0$ Peroxide 97 Di-n-propylamine $C_{6}H_{15}N$ $142-84-7$ Amines 98 Di-n-propyldiazene $C_{6}H_{14}N_{2}O$ $87339-10-4$ Nitroso 102	Diphenylmethane	$C_{13}H_{12}$	101-81-5	Aromat02	875
meso-2,3-Diphenylsuccinic acid $C_{16}H_{14}O_{4}$ 1225-13-4 Acids 96 racemic-2,3-Diphenylsuccinic acid $C_{16}H_{14}O_{4}$ 7584-72-7 Acids 96 Diphenyl sulfide $C_{12}H_{10}S$ 139-66-2 Sulfides 104 Diphenyl sulfone $C_{12}H_{10}O_{2}S$ 127-63-9 Sulfones 105 Diphenyl sulfoxide $C_{12}H_{10}O_{2}S$ 945-51-7 Sulfoxides 105 N,N-Diphenylurea $C_{12}H_{10}O_{2}S$ 945-51-7 Sulfoxides 105 N,N'-Diphenylurea $C_{13}H_{12}N_{2}O$ 603-54-3 Ureas 101 N,N'-Diphenylurea $C_{13}H_{12}N_{2}O$ 102-07-8 Ureas 101 Dipropanoyl peroxide $C_{6}H_{10}O_{4}$ 3248-28-0 Peroxide 97 Dipropionyl peroxide $C_{6}H_{10}O_{4}$ 3248-28-0 Peroxide 97 Di-n-propyldiazene $C_{6}H_{14}N_{2}$ 821-67-0 Diazene 99 Di-n-propyldiazene $C_{6}H_{14}N_{2}O$ 87339-10-4 Nitroso 102	Diphenyl oxide	$C_{12}H_{10}O$	101-84-8	Ethers	935
racemic-2,3-Diphenylsuccinic acid $C_{16}H_{14}O_{4}$ 7584-72-7 Acids 96 Diphenyl sulfide $C_{12}H_{10}S$ 139-66-2 Sulfides 104 Diphenyl sulfone $C_{12}H_{10}O_{2}S$ 127-63-9 Sulfones 105 Diphenyl sulfoxide $C_{12}H_{10}OS$ 945-51-7 Sulfoxides 105 N,N-Diphenylurea $C_{13}H_{12}N_{2}O$ 603-54-3 Ureas 101 N,N'-Diphenylurea $C_{13}H_{12}N_{2}O$ 102-07-8 Ureas 101 Dipropanoyl peroxide $C_{6}H_{10}O_{4}$ 3248-28-0 Peroxide 97 Dipropionyl peroxide $C_{6}H_{10}O_{4}$ 3248-28-0 Peroxide 97 Di-n-propylamine $C_{6}H_{14}N_{2}$ 821-67-0 Diazene 99 Di-n-propyldiazene $C_{6}H_{14}N_{2}O$ 87339-10-4 Nitroso 102	1,3-Diphenyl-1,3-propanedione	$C_{15}H_{12}O_2$	120-467	Ketones	945
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	meso-2,3-Diphenylsuccinic acid	$C_{16}H_{14}O_{4}$	1225-13-4	Acids	963
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	racemic-2,3-Diphenylsuccinic acid	$C_{16}H_{14}O_{4}$	7584-72-7	Acids	963
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Diphenyl sulfide	$C_{12}H_{10}S$	139-66-2		1047
N,N-Diphenylurea $C_{13}H_{12}N_2O$ $603-54-3$ Ureas 101 N,N'-Diphenylurea $C_{13}H_{12}N_2O$ $102-07-8$ Ureas 101 Dipropanoyl peroxide $C_6H_{10}O_4$ $3248-28-0$ Peroxide 97 Dipropionyl peroxide $C_6H_{10}O_4$ $3248-28-0$ Peroxide 97 Di-n-propylamine $C_6H_{15}N$ $142-84-7$ Amines 98 Di-n-propyldiazene $C_6H_{14}N_2$ $821-67-0$ Diazene 99 Di-n-propyldiazene N-oxide (E) $C_6H_{14}N_2O$ $87339-10-4$ Nitroso 102			127-63-9	Sulfones	1054
N,N-Diphenylurea $C_{13}H_{12}N_2O$ 603-54-3 Ureas 101 N,N'-Diphenylurea $C_{13}H_{12}N_2O$ 102-07-8 Ureas 101 Dipropanoyl peroxide $C_6H_{10}O_4$ 3248-28-0 Peroxide 97 Dipropionyl peroxide $C_6H_{10}O_4$ 3248-28-0 Peroxide 97 Di-n-propylamine $C_6H_{15}N$ 142-84-7 Amines 98 Di-n-propyldiazene $C_6H_{14}N_2$ 821-67-0 Diazene 99 Di-n-propyldiazene N-oxide (E) $C_6H_{14}N_2O$ 87339-10-4 Nitroso 102		$C_{12}H_{10}OS$	945-51-7	Sulfoxides	1050
Dipropanoyl peroxide $C_6H_{10}O_4$ 3248–28–0 Peroxide 97 Dipropionyl peroxide $C_6H_{10}O_4$ 3248–28–0 Peroxide 97 Di-n-propylamine $C_6H_{15}N$ 142–84–7 Amines 98 Di-n-propyldiazene $C_6H_{14}N_2$ 821–67–0 Diazene 99 Di-n-propyldiazene N-oxide (E) $C_6H_{14}N_2O$ 87339–10–4 Nitroso 102		$C_{13}H_{12}N_2O$	603-54-3	Ureas	1013
Dipropionyl peroxide $C_6H_{10}O_4$ 3248–28–0 Peroxide 97 Di-n-propylamine $C_6H_{15}N$ 142–84–7 Amines 98 Di-n-propyldiazene $C_6H_{14}N_2$ 821–67–0 Diazene 99 Di-n-propyldiazene N-oxide (E) $C_6H_{14}N_2O$ 87339–10–4 Nitroso 102		$C_{13}H_{12}N_2O$	102-07-8	Ureas	1013
Dipropionyl peroxide $C_6H_{10}O_4$ 3248–28–0 Peroxide 97 Di-n-propylamine $C_6H_{15}N$ 142–84–7 Amines 98 Di-n-propyldiazene $C_6H_{14}N_2$ 821–67–0 Diazene 99 Di-n-propyldiazene N-oxide (E) $C_6H_{14}N_2O$ 87339–10–4 Nitroso 102	Dipropanoyl peroxide	$C_6H_{10}O_4$	3248-28-0	Peroxide	978
Di-n-propylamine $C_6H_{15}N$ 142-84-7 Amines 98 Di-n-propyldiazene $C_6H_{14}N_2$ 821-67-0 Diazene 99 Di-n-propyldiazene N-oxide (E) $C_6H_{14}N_2O$ 87339-10-4 Nitroso 102	Dipropionyl peroxide	$C_6H_{10}O_4$	3248-28-0	Peroxide	978
Di-n-propyldiazene $C_6H_{14}N_2$ 821-67-0 Diazene 99 Di-n-propyldiazene N-oxide (E) $C_6H_{14}N_2$ O 87339-10-4 Nitroso 102			142-84-7		985
Di-n-propyldiazene N-oxide (E) $C_6H_{14}N_2O$ 87339–10-4 Nitroso 102	Di-n-propyldiazene		821670		998
• ••					1022
2.11 p. 2p. 1000	Di-n-propyl disulfide	$C_6H_{14}S_2$	629-19-6	Disulfides	1048

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
Di-n-propyl ether	C ₆ H ₁₄ O	111-43-3	Ethers	926
Di-n-propyl sulfate	$C_6H_{14}O_4S$	598-05-0	Sulfates	1055
Di-n-propyl sulfide	$C_6H_{14}S$	111–47–7	Sulfides	1043
Di-n-propyl sulfite	$C_6H_{14}O_3S$	623-98-3	Sulfites	1055
Di-n-propyl sulfone	$C_6H_{14}O_2S$	598-03-8	Sulfones	1052
Di-n-propyl sulfoxide	$C_6H_{14}OS$	4253–91–2	Sulfoxides	1049,1050
Di-(1,1,3,3-tetramethylbutyl)diazene	$C_{16}H_{34}N_2$	39198-34-0	Diazene	999
Divinyl ether	C₄H ₆ O	109–93–3	Ethers	929
Divinyl sulfone	$C_4H_6O_2S$	77–77–0	Sulfones	1050
3,9-Dodecadiyne	$C_{12}H_{18}$	61827–89–2	Alkynes	862
5,7-Dodecadiyne	$C_{12}H_{18}$	1120-29-2	Alkynes	862
Dodecafluorocyclohexane	C ₆ F ₁₂	355–68–0	Fluoride	1063
Dodecane	$C_{12}H_{26}$	112–40–3	n-Alkanes	831,832
Dodecanedioic acid	$C_{12}H_{22}O_4$	693–23–2	Acids	953
Dodecanoic acid	$C_{12}H_{24}O_2$	143-07-7	Acids	947
Dodecanol	$C_{12}H_{26}O$	112–53–8	Alcohols	911,912
n-Dodecyl alcohol	$C_{12}H_{26}O$	112–53–8	Alcohols	911,912
Dodecylbenzene	$C_{18}H_{30}$	123-01-3	Aromat01	868
Dodecylcyclohexane	C ₁₈ H ₃₆	1795–17–1	Cyclic02	898
Dotriacontane	$C_{32}H_{66}$	544–85–4	n-Alkanes	834
E				
EGDN	$C_2H_4N_2O_6$	628-96-6	Nitrates	1032
Eicosane	$C_{20}H_{42}$	112–95–8	n-Alkanes	833
1-Eicosanethiol	$C_{20}H_{42}S$	13373-97-2	Thiols	1037
Eicosanoic acid	$C_{20}H_{40}O_2$	506–30–9	Acids	949,950
Eicosanol	$C_{20}H_{42}O$	629–96–9	Alcohols	914
n-Eicosanyl alcohol	$C_{20}H_{42}O$	629–96–9	Alcohols	914
Enanthonitrile	$C_7H_{13}N$	629-08-3	Nitriles	993
Enanthylic acid	$C_7H_{14}O_2$	111–14–8	Acids	946
Erythritol	$C_4H_{10}O_4$	149326	Alcohols	919
Ethanal	C₂H₄O	75–07–0	Aldehyde	935
Ethanamide	C₂H₅NO	60-35-5	Amides	1006
Ethane	C_2H_6	74840	n-Alkanes	830
Ethanedial	$C_2H_2O_2$	107–22–2	Aldehyde	935
1,2-Ethanediamine	$C_2H_8N_2$	107–15–3	Amines	983,984
Ethanedioic acid	$C_2H_2O_4$	144–62–7	Acids	951
1,2-Ethanediol	C ₂ H ₄ O ₂	107-21-1	Alcohols	917
1,2-Ethanedithiol	$C_2H_6S_2$	540-63-6	Thiols	1037,1038
Ethanenitrile	C ₂ H ₃ N	75–05–8	Nitriles	992
Ethanethiol	C_2H_6S	75081	Thiols	1035
Ethanoic acid	C₂H₄O₂	64–19–7	Acids	945
Ethanoic anhydride	$C_4H_6O_3$	108-24-7	Anhydrides	964
Ethanol	C ₂ H ₆ O	64–17–5	Alcohols	909
Ethenoxyethene	C₄H ₆ O	109-93-3	Ethers	929
Ethenylcyclopentane	C ₇ H ₁₂	3742–34–5	Cyclic02	895
Ethenyl ethanoate	$C_4H_6O_2$	108-05-4	Esters	971
Ethoxybenzene	$C_8H_{10}O$	103-73-1	Ethers	934
Ethoxyethane	$C_4H_{10}O$	60–29–7	Ethers	926
2-Ethoxyethanol	$C_4H_{10}O_2$	110–80–5	Ethers	931
Ethoxyethene	C_4H_8O	109-92-2	Ethers	929
Ethoxypropane	$C_5H_{12}O$	628-32-0	Ethers	928
N-Ethylacetamide	C ₄ H ₉ NO	625-50-3	Amides	1008
Ethyl acctate	$C_4H_8O_2$	141-78-6	Esters	968,969
Ethyl alcohol	C₂H ₆ O	64–17–5	Alcohols	909
Ethyl amine	C_2H_7N	75–04–7	Amines	982
N-Ethylaniline	$C_8H_{11}N$	103–69–5	Amines	990
Ethylbenzene	C_8H_{10}	100-41-4	Aromat01	866
Ethyl benzoate	$C_9H_{10}O_2$	93–89–0	Esters	976
4-Ethyl benzophenone	$C_{15}H_{14}O$	18220-90-1	Ketones	944
Ethylbutanedioic acid	$C_6H_{10}O_4$	636-48-6	Acids	955
2-Ethyl-1-butene	C_6H_{12}	760–21–4	s-Alkenes	852,853
Ethyl (E)-2-butenoate	$C_6H_{10}O_2$	623-70-1	Esters	972
Ethyl trans-2-butenoate	$C_6H_{10}O_2$	623–70–1	Esters	972
Ethyl tert-butyl ketone	$C_7H_{14}O$	564045	Ketones	941

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
Ethyl 4-chlorobutanoate	C ₆ H ₁₁ ClO ₂	3153-36-4	Chloride	1082
Ethyl 2-chloropropanoate	$C_5H_9ClO_2$	535-13-7	Chloride	1081
Ethylcyclobutane	C_6H_{12}	4806–61–5	Cyclic01	891
Ethylcyclohexane	C ₈ H ₁₆	1678–91–7	Cyclic02	897
1-Ethylcyclohexene	C ₈ H ₁₄	1453–24–3	Cyclic02	899
Ethylcyclopentane	C ₇ H ₁₄	1640–89–7	Cyclic01	892
1-Ethylcyclopentene	C ₇ H ₁₂	2146–38–5	Cyclic02	896
Ethyl 2,3-dichloropropanoate	C ₅ H ₈ Cl ₂ O ₂	6628–21–3	Chloride	1083
2-Ethyl-1,4-dimethylbenzene	$C_{10}H_{14}$	1758–88–9	Aromat01	870
2-Ethyl-1,3-dimethylbenzene	$C_{10}H_{14}$	2870-04-4	Aromat01	870
3-Ethyl-1,2-dimethylbenzene	$C_{10}H_{14}$	933-98-2	Aromat01	869
4-ethyl-1,2-dimethylbenzene	C ₁₀ h ₁₄	934–80–5	Aromat01	870
4-Ethyl-1,3-dimethylbenzene	$C_{10}H_{14}$	874-41-9	Aromat01	870
5-Ethyl-1,3-dimethylbenzene	C ₁₀ H ₁₄	934-74-7	Aromat01	870
N'-Ethyl-N,N-diphenylurea	C ₁₅ H ₁₆ N ₂ O	18168-01-9	Ureas	1013
Ethylene Ethylene explanate	C₂H₄	74-85-1	n-Alkenes	846
Ethylene carbonate	C ₃ H ₄ O ₃	96-49-1	Carbonates	982
Ethylenediamine	C ₂ H ₈ N ₂ C ₂ H ₆ N₄O₄	107-15-3 26958-29-2	Amines	983,984
Ethylene dinitramine Ethylene glycol		26938-29-2 107-21-1	Nitramines	1033
Ethylene glycol dinitrate	C ₂ H ₆ O ₂	628-96-6	Alcohols	917
	$C_2H_4N_2O_6$		Nitrates	1032
Ethyleneimine	C₂H₅N C₂H₄O	151-56-4 75-21-8	CyclCHN	1001
Ethylene oxide N-Ethylethanamide	C ₄ H ₉ NO	627-45-2	Ethers	932
Ethyl ethanoate	C ₄ H ₈ O ₂	141-78-6	Amides Esters	1008
Ethyl formate	C ₃ H ₆ O ₂	109-94-4	Esters	968,969
3-Ethylheptane	C ₃ H ₂₀	15869-80-4	t-Alkanes	968
4-Ethylheptane	C ₉ H ₂₀	2216-32-2	t-Alkanes	839
2-Ethylhexanal	C ₈ H ₁₆ O	123-05-7	Aldehyde	839
3-Ethylhexane	C ₈ H ₁₈	619-99-8	t-Alkanes	937
2-Ethyl-1-hexanol	C*H18O	104-76-7	Alcohols	839 915
Ethyl hexyl sulfide	C ₈ H ₁₈ S	7309-44-6	Sulfides	1045
Ethylidenecyclohexane	C ₈ H ₁₄	1003-64-1	Cyclic02	899
Ethylidenecyclopentane	C_7H_{12}	2146-37-4	Cyclic02	894,895
Ethyl isopropyl ketone	C ₆ H ₁₂ O	565-69-5	Ketones	941
Ethyl methanoate	$C_3H_6O_2$	109-94-4	Esters	968
Ethyl 2-methylbutanoate	$C_7H_{14}O_2$	7452-79-1	Esters	908 971
1-Ethyl-1-methylcyclopentane	C ₈ H ₁₆	16747–50–5	Cyclic03	
cis-1-Ethyl-2-methylcyclopentane	C ₈ H ₁₆	930-89-2	Cyclic03	905,906 905
trans-1-Ethyl-2-methylcyclopentane	C ₈ H ₁₆	930–90–5	Cyclic03	905
cis-1-Ethyl-3-methylcyclopentane	C ₈ H ₁₆	2613-66-3	Cyclic03	905
trans-1-Ethyl-3-methylcyclopentane	C ₈ H ₁₆	2613-65-2	Cyclic03	905
2-Ethyl-3-methylnaphthalene	C ₁₃ H ₁₄	31032-94-7	Aromat02	903 884
2-Ethyl-6-methylnaphthalene	C ₁₃ H ₁₄	7372–86–3	Aromat02	884
2-Ethyl-7-methylnaphthalene	C ₁₃ H ₁₄	17059-55-1	Aromat02	884
3-Ethyl-2-methylpentane	C ₈ H ₁₈	609–26–7	t-Alkanes	841
3-Ethyl-3-methylpentane	C_8H_{18}	1067-08-9	q-Alkanes	845
Ethyl methyl sulfide	C₃H ₈ S	624-89-5	Sulfides	1041
Ethyl methyl sulfite	C ₃ H ₈ O ₃ S	10315-59-0	Sulfites	1055
Ethyl methyl sulfone	$C_3H_8O_2S$	594-43-4	Sulfones	1050
1-Ethylnaphthalene	$C_{12}H_{12}$	1127–76–0	Aromat02	880
2-Ethylnaphthalene	$C_{12}H_{12}$	939–27–5	Aromat02	880
Ethyl nitrate	C ₂ H ₅ NO ₃	625-58-1	Nitrates	1032
Ethyl nitrite	$C_2H_5NO_2$	109-95-5	Nitrites	1031
3-Ethyloctane	$C_{10}H_{22}$	5881-17-4	t-Alkanes	839
4-Ethyloctane	$C_{10}H_{22}$	15869-86-0	t-Alkanes	839
Ethyl-2,4-pentadienoate	$C_7H_{10}O_2$	13038-12-5	Esters	973
3-Ethylpentane	C ₇ H ₁₆	617–78–7	t-Alkanes	838
Ethyl pentanoate	$C_7H_{14}O_2$	539-82-2	Esters	970
Ethyl cis-2-pentenoate	$C_7H_{12}O_2$	27805-84-1	Esters	972
Ethyl trans-2-pentenoate	$C_7H_{12}O_2$	24410-84-2	Esters	972
Ethyl (E)-2-pentenoate	$C_7H_{12}O_2$	24410-84-2	Esters	972
Ethyl cis-3-pentenoate	$C_7H_{12}O_2$	27829-70-5	Esters	972 972
Ethyl trans-3-pentenoate	$C_7H_{12}O_2$	3724-66-1	Esters	972,973
		212T-00-1	Library 19	717.713
Ethyl (E)-3-pentenoate	$C_7H_{12}O_2$	3724-66-1	Esters	972,973

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
Ethyl (Z)-3-pentenoate	C ₇ H ₁₂ O ₂	27829-70-5	Esters	972
Ethyl 4-pentenoate	$C_7H_{12}O_2$	1968-40-7	Esters	973
Ethyl pentyl sulfide	$C_7H_{16}S$	26158-99-6	Sulfides	1043,1044
Ethyl-3-pentynoate	$C_7H_{10}O_2$	52750-56-8	Esters	972
Ethyl-4-pentynoate	$C_7H_{10}O_2$	63093-41-4	Esters	972
2-Ethylphenol	$C_8H_{10}O$	90006	Alcohols	922
3-Ethylphenol	$C_8H_{10}O$	620–17–7	Alcohols	922
4-Ethylphenol	$C_8H_{10}O$	123-07-9	Alcohols	922
Ethyl phenyl ether	$C_8H_{10}O$	103-73-1	Ethers	934
Ethyl phenyl ketone	$C_9H_{10}O$	93550	Ketones	944
Ethyl phenyl sulfide	$C_8H_{10}S$	622-38-8	Sulfides	1047
Ethyl propanoate	$C_5H_{10}O_2$	105-37-3	Esters	970
3-Ethyl-1-propene sulfide	C ₅ H ₁₀ S	5296-62-8	Sulfides	1046
Ethyl propionate	$C_5H_{10}O_2$	105-37-3	Esters	970
	$C_5H_{10}O_2$ $C_5H_{12}O$	628-32-0	Ethers	
Ethyl propyl ether				928
Ethyl propyl ketone	$C_6H_{12}O$	589-38-8	Ketones	939
Ethyl propyl sulfide	$C_5H_{12}S$	4110–50–3	Sulfides	1042
Ethylsuccinic acid	$C_6H_{10}O_4$	636–48–6	Acids	955
Ethylurea	$C_3H_8N_2O$	625-52-5	Ureas	1011
Ethyl valerate	$C_7H_{14}O_2$	539-82-2	Esters	970
Ethyl sec-valerate	$C_7H_{14}O_2$	7452-79-1	Esters	971
Ethyl vinyl ether	C_4H_8O	109-92-2	Ethers	929
Ethynylbenzene	C_8H_6	536-74-3	Aromat02	874,875
F				
Fluoranthrene	$C_{16}H_{10}$	206-44-0	Aromat02	886
Fluorobenzene	C ₆ H ₅ F	462066	Fluoride	1060
2-Fluorobenzoic acid	C ₇ H ₅ FO ₂	445-29-4	Fluoride	1065
3-Fluorobenzoic acid	$C_7H_5FO_2$	455-38-9	Fluoride	1065
4-Fluorobenzoic acid	C ₇ H ₅ FO ₂	456-22-4	Fluoride	1065
Fluoroethane	C ₂ H ₅ F	353-36-6	Fluoride	1058
Fluoroethylene	C ₂ H ₃ F	75-02-5	Fluoride	1059
Fluoromethane	CH₃F	593-53-3	Fluoride	1058
1-Fluoro-4-methylbenzene	C ₇ H ₇ F	352–32–9	Fluoride	1060,1061
1-Fluoropropane	C₃H₁F	460–13–9	Fluoride	1058
2-Fluoropropane	C_3H_7F	420-26-8	Fluoride	1058
p-Fluorotoluene	C ₇ H ₇ F	352-32-9	Fluoride	1060,1061
		401-80-9	Fluoride	•
1-Fluoro-3-(trifluoromethyl)benzene	C ₇ H ₄ F ₄			1062
Formaldehyde	CH ₂ O	50-00-0	Aldehyde	935
Formamide	CH₃NO	75–12–7	Amides	1006
Formic acid	CH_2O_2	64–18–6	Acids	945
Fumaric acid	C ₄ H ₄ O ₄	110–17–8	Acids	951
Furan	C₄H₄O	110-00-9	Ethers	933
Furfural	$C_5H_4O_2$	98–01–1	Aldehyde	938
G				
L-Glutamic acid	C5H9NO4	56–86-0	Amino acids	1018
L-Glutamine	$C_5H_{10}N_2O_3$	56-85-9	Amino acids	1018
Glutaric acid	C₅H ₈ O ₄	110–94–1	Acids	952
Glutaric anhydride	$C_5H_6O_3$	108-55-4	Anhydrides	964
Glutarimide	C ₅ H ₇ NO ₂	1121-89-7	CyclCHNO	1035
Glutaronitrile	$C_5H_6N_2$	544-13-8	Nitriles	996
Glycerol	C ₃ H ₈ O ₃	56-81-5	Alcohols	918
Glycerol Glyceryl trinitrate	C ₃ H ₅ N ₃ O ₉	55-63-0	Nitrates	1033
		56-40-6		1014
Glycine	C ₂ H ₅ NO ₂		Amino acids	
Glycylalanylphenylalanine	C ₁₄ H ₁₉ N ₃ O ₄	17922-87-1	Amino acids	1021
Glycylglycine	$C_4H_8N_2O_3$	556–50–3	Amino acids	1019
Glycylphenylalanine	$C_{11}H_{14}N_2O_3$	3321-03-7	Amino acids	1020
N-Glycyl-DL-valine	$C_7H_{14}N_2O_3$	2325-17-9	Amino acids	1020
Glyoxal	$C_2H_2O_2$	107–22–2	Aldehyde	935
н				
Haleite	$C_2H_4N_4O_4$	26958–29–2	Nitramines	1033

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
leptadecane	C ₁₇ H ₃₆	629-78-7	n-Alkanes	8:
Ieptadecanoic acid	$C_{17}H_{34}O_2$	506-12-7	Acids	94
Ieptadecanol	C ₁₇ H ₃₆ O	123-24-0	Alcohols	9
-Heptadecyl alcohol	C ₁₇ H ₃₆ O	123-24-0	Alcohols	91
2,2,3,3,4,4,4-Heptafluoro-1-butanol	C ₄ H ₃ F ₇ O	375-01-9	Fluoride	100
leptaldehyde .	$C_7H_{14}O$	111-71-7	Aldehyde	936,93
Teptanal	C7H14O	111-71-7	Aldehyde	936,93
Heptane	C7H16	142-82-5	n-Alkanes	830,83
Heptanedioic acid	C ₇ H ₁₂ O ₄	111-16-0	Acids	9
1-Heptanethiol	$C_7H_{16}S$	1639-09-4	Thiols	103
Heptanenitrile	$C_7H_{13}N$	629-08-3	Nitriles	99
Teptanoic acid	C ₂ H ₁₄ O ₂	111-14-8	Acids	94
Heptanol	C ₂ H ₁₆ O	111-70-6	Alcohols	910,91
-Heptene	C ₇ H ₁₄	592-76-7	n-Alkenes	84
is-2-Heptene	C ₇ H ₁₄	6443-92-1	n-Alkenes	84
rans-2-Heptene	C ₇ H ₁₄	14686-13-6 7642-10-6	n-Alkenes	84
is-3-Heptene	C ₇ H ₁₄		n-Alkenes	85
rans-3-Heptene	C ₇ H ₁₄	14686-14-7	n-Alkenes	85
-Heptyl alcohol	C ₇ H ₁₆ O	111-70-6	Alcohols	910,91
Heptylbenzene	C13H20	1078-71-3 5617-41-4	Aromat01	80
Heptylcyclohexane	C ₁₃ H ₂₆	5617-42-5	Cyclic03	90
leptylcyclopentane	C ₁₂ H ₂₄		Cyclic02	89
-Heptyl-1-hydroperoxide	C ₇ H ₁₆ O ₂	764-81-8	Hydroperoxides	97
-Heptyl-2-hydroperoxide	$C_7H_{16}O_2$	762-46-9 761-70-6	Hydroperoxides	97
-Heptyl-3-hydroperoxide	C ₇ H ₁₆ O ₂		Hydroperoxides	98
-Heptyl-4-hydroperoxide	C ₇ H ₁₆ O ₂	761-40-0	Hydroperoxides	98
leptyl methyl sulfide	C ₈ H ₁₈ S	20291-61-6	Sulfides	10-
-Heptyne	C ₇ H ₁₂ C ₆ Cl ₆	628-71-7	Alkynes	8.
lexachlorobenzene		118-74-1	Chloride	107
Texachloroethane	C ₂ Cl ₆	67-72-1 630-01-3	Chloride	107
Hexacosane	C26H54 C7F10		n-Alkanes	83
Hexadecafluoroheptane Hexadecane	C ₁₆ H ₃₄	335-57-9 544-76-3	Fluoride	105
-Hexadecanethiol	C ₁₆ H ₃₄ S		n-Alkanes	83
-riexadecaneitmoi Hexadecanoic acid		2917-26-2 57-10-3	Thiols	103
	C ₁₆ H ₃₂ O ₂		Acids	948,94
Hexadeconol -Hexadecone	C16H34O	36653824 629732	Alcohois	91
-Hexadecyl alcohol	C10H32 C16H34O		n-Alkenes	64
-Hexadecyne		36653-82-4 629-74-3	Alcohols	91
	C ₁₆ H ₃₀		Alkynes	86
,S-Hexadiyne	C ₆ H ₆	628-16-0	Alkynes	86
łexaethylbenzene łexafluorobenzene	C ₁₈ H ₃₀	604-88-6	Aromat02	87
texanuorobenzene Lexafluoroethane	C ₆ F ₆	392-56-3	Fluoride	106
	C₂F ₆	76–16–4	Fluoride	105
is-Hexahydroindan	C ₃ H ₁₆	4551-51-3	Cyclic02	90
uns-Hexahydroindan	C ₄ H ₁₆	3296-50-2	Cyclic02	90
lexaldehyde	C ₆ H ₁₂ O	66-25-1	Aldehyde	93
Iexamethylbenzene	C ₁₂ H ₁₈	87-85-4	Aromat01	86
lexamethyleneimine	C ₆ H ₁₃ N	111-49-9	CyclCHN	100
lexanal	C ₆ H ₁₂ O	66-25-1	Aldehyde	93
lexanamide	C ₆ H ₁₃ NO	628-02-4	Amides	1007,100
lexane	C_6H_{14}	110-54-3	n-Alkanes	83
6-Hexanedinitrile	C ₆ H ₈ N ₂	111-69-3	Nitriles	99
lexanedioic acid	C,H10O4	124-04-9	Acids	9:
6-Hexanediol	$C_6H_{14}O_2$	629-11-8	Alcohols	9
Hexanethiol	C ₆ H ₁₄ S	111-31-9	Thiols	10
lexanoic acid	C ₆ H ₁₂ O ₂	142-62-1	Acids	9
lexanol	C4H14O	111-27-3	Alcohols	9
-Hexanol	C ₆ H ₁₄ O	626-93-7	Alcohols	9:
Hexanol	$C_6H_{14}O$	623-37-0	Alcohols	9:
lexanolactone	$C_6H_{10}O_2$	502-44-3	Esters	9
Hexanone	$C_6H_{12}O$	591786	Ketones	92
Hexanone	$C_6H_{12}O$	589-38-8	Ketones	93
lexaphenylethane	C38H30	17854-07-8	Cyclic03	90
-Hexene	C ₆ H ₁₂	592-41-6	n-Alkenes	84

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
trans-2-Hexene	C ₆ H ₁₂	4050–45–7	n-Alkenes	848
cis-3-Hexene	C_6H_{12}	7642-09-3	n-Alkenes	848,849
trans-3-Hexene	C_6H_{12}	13269-52-8	n-Alkenes	849
Hexogen	C ₃ H ₆ N ₆ O ₆	121-82-4	Nitramin	1034
n-Hexyl alcohol	$C_6H_{14}O$	111–27–3	Alcohols	910
n-Hexyl amine	$C_6H_{15}N$	111-26-2	Amines	983
Hexylbenzene	$C_{12}H_{18}$	1077–16–3	Aromat01	866
Hexylcyclopentane	C ₁₁ H ₂₂	4457–00–5	Cyclic02	893,894
n-Hexyl-1-hydroperoxide	C ₆ H ₁₄ O ₂	4312–76–9	Hydroperoxides	979
n-Hexyl-2-hydroperoxide	$C_6H_{14}O_2$	24254–55–5	Hydroperoxides	979
n-Hexyl-3-hydroperoxide	$C_6H_{14}O_2$	24256-56-6		
			Hydroperoxides	979
Hexyl methyl sulfide	C ₇ H ₁₆ S	20291-60-5	Sulfides	1044
1-Hexyne	C_6H_{10}	693-02-7	Alkynes	859
Hippuric acid	C ₉ H ₉ NO ₃	495–69–2	Amino acids	1019
Hippurylglycine	$C_{11}H_{12}N_2O_4$	1145-32-0	Amino acids	1020
HMX	$C_4H_8N_8O_8$	2691–41–0	Nitramines	1034
Hydrazine	N_2H_4	302-01-2	Hydrazines	997
Hydrazobenzene	$C_{12}H_{12}N_2$	122–66–7	Hydrazines	998
Hydroquinonc	$C_6H_6O_2$	123-31-9	Alcohols	924
DL-3-Hydroxy-2-aminobutanoic acid	C ₄ H ₉ NO ₃	80682	Amino acids	1017
DL-3-Hydroxy-2-aminopropanoic acid	C ₃ H ₇ NO ₃	302-84-1	Amino acids	1017
2-Hydroxybenzoic acid	$C_7H_6O_3$	69–72–7	Acids	961
3-Hydroxy-2-naphthoic acid	$C_{11}II_8O_3$	7584–72–7	Acids	963
L-2-Hydroxypropanoic acid	$C_3H_6O_3$	79-33-4	Acids	946
I				
Indane	C ₂ H ₁₀	496–11–7	Cyclic02	901
Indene			- · · · · · · · · · · · · · · · · · · ·	
	C₃H ₈	95-13-6	Cyclic02	902
Iodobenzene	C ₆ H ₅ I	591–50–4	Iodide	1094
2-Iodobenzoic acid	C ₇ H ₅ IO ₂	88–67–5	Iodide	1097
3-Iodobenzoic acid	C ₇ H ₅ IO ₂	618–51–9	Iodide	1098
4-Iodobenzoic acid	$C_7H_5IO_2$	619-58-9	Iodide	1098
Iodocyclohexane	$C_6H_{11}I$	626-62-0	Iodide	1096
Iodoethane	C₂H ₅ I	75-03-6	Iodide	1092
Iodomethane	CH₃I	74-88-4	Iodide	1092
1-Iodo-2-methylbenzene	C ₇ H ₇ I	615-37-2	Iodide	1095
1-Iodo-3-methylbenzene	C ₇ H ₇ I	625-95-6	Iodide	1095
1-Iodo-3-methylbutane	$C_5H_{11}I$	541-28-6	Iodide	1093
1-Iodo-4-methylbenzene	C ₇ H ₇ I	624–31–7	Iodide	1095
1-Iodo-2-methylpropane	C ₄ H ₉ I	513-38-2	Iodide	1093
2-Iodo-2-methylpropane	C ₄ H ₉ I	558-17-8	Iodide	1093
1-Iodonaphthalene	C ₁₀ H ₇ I	90-14-2	Iodide	1095
2-Iodonaphthalene	C ₁₀ H ₇ I	612–55–5	Iodide	1095
Iodopentafluorobenzene	C ₆ F ₅ I	827–15–6	Mixed	1101
2-Iodophenol	C₀H₅IO	533-58-4	Iodide	1097
3-Iodophenol	C ₆ H ₅ IO	626028	Iodide	1097
4-Iodophenol	C ₆ H ₅ IO	540–38–5	Iodide	1097
1-Iodopropane	C_3H_7I	107-08-4	Iodide	1092
2-Iodopropane	C ₃ H ₇ I	75–30–9	Iodide	1093
3-Iodopropanoic acid	C ₃ H ₅ IO ₂	141-76-4	Iodide	1097
1-Iodo-1-propene (E)	C ₃ H ₅ I	7796–54–5	Iodide	1094
1-Iodo-1-propene (Z)	C ₃ H ₅ I	7796–36–3	Iodide	1094
3-Iodo-1-propene	C ₃ H ₅ I	556-56-9	Iodide	1094
1-Iodopropyne	C ₃ H ₃ I	624–66–8	Iodide	1094
Isoamyl alcohol	C ₅ H ₁₂ O	123-51-3	Alcohols	914
Isobutyl acetate				
•	$C_6H_{12}O_2$	110–19–0	Esters	969
Isobutyl alcohol	C ₄ H ₁₀ O	78–83–1	Alcohols	914
Isobutyl amine	C ₄ H ₁₁ N	78-81-9	Amines	983
Isobutylbenzene	$C_{10}H_{14}$	538-93-2	Aromat02	873
Isobutyl formate	$C_5H_{10}O_2$	542-55-2	Esters	969
Isobutyraldehyde	C_4H_8O	78-84-2	Aldehyde	937
Isobutyronitrile	C_4H_7N	78-82-0	Nitriles	994
DL-Isoleucine	$C_6H_{13}NO_2$	443–79–8	Amino acids	1016
······································				
Isophthalic acid	$C_8H_6O_4$	121-91-5	Acids	962

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
2-Isopropoxyethanol	C ₅ H ₁₂ O ₂	109-59-1	Ethers	932
N-Isopropylacetamide	C₅H ₁₁ NO	1118 -69-0	Amides	1008
Isopropyl acetate	$C_5H_{10}O_2$	108-21-4	Esters	969
Isopropyl alcohol	C₃H ₈ O	67-63-0	Alcohols	915
Isopropyl amine	C ₃ H ₉ N	75-31-0	Amines	984
Isopropylbenzene	C ₉ H ₁₂	98-82-8	Aromat02	872
Isopropylbiphenyl	C ₁₅ H ₁₆	7116-95-2	Aromat02	879
Isopropyl (E)-2-butenoate	$C_7H_{12}O_2$	18060-77-0	Esters	973
Isopropyl trans-2-butenoate	$C_7H_{12}O_2$	18060-77-0	Esters	973
Isopropyl tert-butyl ether	C ₇ H ₁₆ O	17348-59-3	Ethers	929
Isopropyl tert-butyl ketone	C ₈ H ₁₆ O	5857 - 36 - 3	Ketones	941
Isopropyl ethanoate	$C_5H_{10}O_2$	108-21-4	Esters	969
Isopropyl ethyl sulfide	C ₅ H ₁₂ S	5145-99-3	Sulfides	1046
4-Isopropylheptane	$C_{10}H_{22}$	52896-87-4	t-Alkanes	840
Isopropyl methyl sulfide	C ₄ H ₁₀ S	1551-21-9	Sulfides	1042
Isopropyl methyl sulfone	$C_4H_{10}O_2S$	4853-74-1	Sulfones	1051
Isopropyl nitrate	$C_3H_7NO_3$	1712-64-7	Nitrates	
		62030-41-5	Esters	1032
Isopropyl 3-pentenoate	$C_8H_{14}O_2$			974
N-Isopropylurea	$C_4H_{10}N_2O$	691–60–1	Ureas	1012
J,K,L				
L-Lactic acid	C ₃ H ₆ O ₃	79-33-4	Acids	946
Lauric acid	$C_{12}H_{24}O_2$	143-07-7	Acids	947,948
DL-Leucine	$C_6H_{13}NO_2$	328-39-2	Amino acids	1016
DL-Leucylglycine	$C_8H_{16}N_2O_3$	615-82-7	Amino acids	1020
2,3-Lutidine	C7H9N	583-61-9	CyclCHN	1004
2,4-Lutidine	C ₇ H ₉ N	108-47-4	CyclCHN	1005
2,5-Lutidine	C ₇ H ₉ N	589-93-5	CyclCHN	1005
2,6-Lutidine	C ₇ H ₉ N	108-48-5	CyclCHN	1005
3,4-Lutidine	C ₇ H ₉ N	583-58-4	CyclCHN	1005
3,5-Lutidine	C ₂ H ₉ N	591-22-0	CyclCHN	1005
DL-Lysine	$C_6H_{14}N_2O_2$	70-54-2	Amino acids	1017
M				
Maleic acid	C₄H₄O₄	110–16–7	Acids	951
Malonamide	$C_3H_6N_2O_2$	108-13-4	Amides	1010
Malonic acid	C ₃ H ₄ O ₄	141-82-2	Acids	951
Margaric acid	C ₁₇ H ₂₄ O ₂	506-12-7	Acids	949
MEDINA	CH ₄ N ₄ O ₄	14168-44-6	Nitramines	1033
2,2-Metacyclophane	C ₁₆ H ₁₆	2319–97–3	Cyclic02	901
2,2-Metaparacyclophane	C ₁₆ H ₁₆	5385-36-4	Cyclic02	
Methanal	CH ₂ O	50-00-0	•	901
Methanamide	CH ₄ NO	75-12-7	Aldehyde Amides	935
Methane	CH ₄	74-82-8		1006
Methanethiol	<u>-</u>	74-62-6 74-93-1	n-Alkanes	830
	CH₄S		Thiols	1035
Methanoic acid	CH ₂ O ₂	64–18–6	Acids	945
Methanol	CH₄O	67–56–1	Alcohols	909
Methoxybenzene	C_7H_8O	100-66-3	Ethers	934
2-Methoxybenzoic acid	$C_8H_8O_3$	579-75-9	Acids	963
3-Methoxybenzoic acid	$C_8H_8O_3$	586-38-9	Acids	963
4-Methoxybenzoic acid	C ₈ H ₈ O ₃	100-09-4	Acids	963
Methoxybutane	$C_5H_{12}O$	628-28-4	Ethers	927
Methoxydecane	C ₁₁ H ₂₄ O	7289-52-3	Ethers	927
Methoxyethane	C₃H ₈ O	540-67-0	Ethers	927
2-Methoxyethanol	$C_3H_8O_2$	109-86-4	Ethers	931
Methoxymethane	C ₂ H ₆ O	115-10-6	Ethers	926
1-Methoxy-3-methylbenzene	C ₈ H ₁₀ O	100-84-5	Ethers	
2-Methoxy-(2-methyl)propane	C ₅ H ₁₂ O	1634-04-4		934
Mcthoxyropane	C₃H₁υO		Ethers	928
		557–17–5 500 52 0	Ethers	927
2-Methoxypropane	C₄H ₁₀ O	598-53-8	Ethers	927,928
Methyl acetate	C ₃ H ₆ O ₂	79–20–9	Esters	966
Methyl acrylate	$C_4H_6O_2$	96–33–3	Esters	971
Methyl alcohol Methyl amine	CH₄O CH₅N	67-56-1 74-89-5	Alcohols Amines	909

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TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Pag
Methylaniline	C7H9N	95–53–4	Amines	9
Methylaniline	C7H9N	108-44-1	Amines	9
Methylaniline	C_7H_9N	106-49-0	Amines	9
-Methylaniline	C ₇ H ₉ N	100–61–8	Amines	9
lethyl azoethane	$C_3H_8N_2$	3880-48-6	Diazene	9
lethyl benzoate	$C_8H_8O_2$	93–58–3	Esters	9
Methyl benzoic acid	$C_8H_8O_2$	118-90-1	Acids	9.
Methyl benzoic acid	$C_8H_8O_2$	99-04-7	Acids	9:
Methyl benzoic acid	$C_8H_8O_2$	99-94-5	Acids	9:
Methylbenzophenone	$C_{14}H_{12}O$	134-84-9	Ketones	94
lethyl benzyl ketone	C ₉ H ₁₀ O	103–79–7	Ketones	9.
-Methylbicyclo[4.1.0]heptane	C ₈ H ₁₄	2439-79-4	Cyclic03	9
Methylbicyclo[2.2.1]hept-2-ene	C ₈ H ₁₂	694–92–8	Cyclic03	9
Methylbicyclo[3.1.0]hexane	C ₇ H ₁₂	4625-24-5	Cyclic03	9
Methylbiphenyl	$C_{13}H_{12}$	643–58–3	Aromat02	8
Methylbiphenyl	$C_{13}H_{12}$	643-93-6	Aromat02	8
Methylbiphenyl	$C_{13}H_{12}$	644-08-6	Aromat02	8
lethyl bromide	CH ₃ Br	74–83–9	Bromide	10
Methyl-1,3-butadiene	C₅H ₈	78–79–5	s-Alkenes	8
Methyl-1,2-butadiene	C ₅ H ₈	598 – 25 – 4	s-Alkenes	8
Methylbutane	C ₅ H ₁₂	78-78-4	t-Alkanes	- 8
•		498-21-5	Acids	
lethylbutanedioic acid	C₃H ₈ O₄			9
Methyl-1-butanethiol	C ₅ H ₁₂ S	1878-18-8	Thiols	10
Methyl-2-butanethiol	C ₅ H ₁₂ S	1679-09-0	Thiols	10
Methyl-1-butanethiol	C ₅ H ₁₂ S	541–31–1	Thiols	10
Methyl-2-butanethiol	C ₅ H ₁₂ S	2084–18–6	Thiols	10
ethyl butanoate	$C_5H_{10}O_2$	623-42-7	Esters	9
Methylbutanoic acid	$C_5H_{10}O_2$	116-53-0	Acids	9
Methylbutanoic acid	$C_5H_{10}O_2$	503-74-2	Acids	9
Mcthyl-1-butanol	C ₅ II ₁₂ O	137–32–6	Alcohols	9
Methyl-1-butanol	C ₅ H ₁₂ O	123–51–3	Alcohols	9
Methyl-2-butanol	$C_5H_{12}O$	75–85–4	Alcohols	9
Methyl-2-butanone	$C_5H_{10}O$	563-80-4	Ketones	9
Methyl-1-butene	C_5H_{10}	563-46-2	s-Alkenes	. 8
Methyl-2-butene	C_5H_{10}	513-35-9	s-Alkenes	. 8
Methyl-1-butene	C5H10	563-45-1	s-Alkenes	8
ethyl (E)-2-butenoate	C ₅ H ₈ O ₂	623-43-8	Esters	9
lethyl trans-2-butenoate	C ₅ H ₈ O ₂	623-43-8	Esters	9
Methyl-4-(1-butenylsulfonyl)benzene	$C_{11}H_{14}O_2S$	111895-49-9	Sulfones	10
Methyl-4-(2-butenylsulfonyl)benzene	$C_{11}H_{14}O_2S$	24931-66-6	Sulfones	10
Methyl-4-(3-butenylsulfonyl)benzene	C ₁₁ H ₁₄ O ₂ S	17482-19-8	Sulfones	10
Methylbutyl 2-chloropropanoate	C ₈ H ₁₅ ClO ₂	62108-69-4	Chloride	10
Methylbutyl 3-chloropropanoate	C ₈ H ₁₅ ClO ₂	62108-70-7	Chloride	10
ethyl-n-butyldiazene	$C_5H_{12}N_2$	4426-46-4	Diazene	ç
Methylbutyl dichloroacetate	C ₇ H ₁₂ Cl ₂ O ₂	37587-83-0	Chloride	10
ethyl butyl ether	C ₅ H ₁₂ O	628-28-4	Ethers	9
ethyl tert-butyl ether	C ₅ H ₁₂ O	1634-04-4	Ethers	9
ethyl butyl ketone		591-78-6	Ketones	9
	C ₆ H ₁₂ O			
ethyl tert-butyl ketone	C ₆ H ₁₂ O	75-97-8	Ketones	9
Methyl-1-butyne	C₃H ₈	598-23-2	Alkynes	. 8
ethyl butyrate	C ₅ H ₁₀ O ₂	623-42-7	Esters	9
ethyl caprate	$C_{11}H_{22}O_2$	1623-43-8	Esters	9
ethyl caproate	$C_7H_{14}O_2$	106–70–7	Esters	9
ethyl caprylate	$C_9H_{18}O_2$	111–11–5	Esters	9
ethyl chloride	CH₃Cl	74–87–3	Chloride	10
ethyl crotonate	$C_5H_8O_2$	623-43-8	Esters	ç
ethylcyclobutane	C_5H_{10}	598618	Cyclic01	8
ethylcyclohexane	C_7H_{14}	108–87–2	Cyclic02	. 8
Methylcyclohexene	C_7H_{12}	591-49-1	Cyclic02	8
ethylcyclopentane	C_6H_{12}	96–37–7	Cyclic01	
Methylcyclopentene	C ₆ H ₁₀	693-89-0	Cyclic02	8
Methylcyclopentene	C_6H_{10}	1120-62-3	Cyclic02	895,8
Methylcyclopentene	C ₆ H ₁₀	1759-81-5	Cyclic02	8
Methyldecane	$C_{11}H_{24}$	6975–98–0	t-Alkanes	. 8
ethyl decanoate	$C_{11}H_{22}O_2$	110-42-9	Esters	9
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TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
Methyl 2,2-dimethylpropanoate	C ₆ H ₁₂ O ₂	598-98-1	Esters	971
Methyldinitramine	CH ₃ N ₃ O ₄	25346-05-8	Nitramines	1033
4-Methyldiphenylmethane	$C_{14}H_{14}$	620-83-7	Aromat02	875
N'-Methyl-N,N-diphenylurea	$C_{14}H_{14}N_2O$	13114-72-2	Ureas	1013
Methyl dodecanoate	$C_{13}H_{26}O_2$	111-82-0	Esters	967
Methyl n-dodecyl ketone	$C_{14}H_{28}O$	2345–27–9	Ketones	940
Methyl enanthate	$C_8H_{16}O_2$	106-73-0	Esters	967
2-Methylenebicyclo[2.2.1]heptane	C_8H_{12}	497-35-8	Cyclic03	904
N,N'-Methylene-bis- $(N,N'$ -dimethylurea)	$C_7H_{16}N_4O_2$	60913-23-7	Ureas	1014
Methylenecyclobutane	C_5H_8	1120-56-5	Cyclic01	891
Methylenecyclohexane	C_7H_{12}	1192-37-6	Cyclic02	896
Methylenecyclopentane	C_6H_{10}	1528-30-9	Cyclic01	891
Methylenedinitramine	CH ₄ N ₄ O ₄	14168-44-6	Nitramines	1033
Methyl ethanoate	$C_3H_6O_2$	79–20–9	Esters	966
1-Methyl-2-ethylbenzene	C ₉ H ₁₂	611–14–3	Aromat01	868
1-Methyl-3-ethylbenzene	C ₉ H ₁₂	620-14-4	Aromat01	868
1-Methyl-4-ethylbenzene	C ₉ H ₁₂	622-96-8	Aromat01	868
3-Methyl-2-ethyl-1-butene	C ₇ H ₁₄	7357–93–9	s-Alkenes	
• •			Diazene	857
Methylethyldiazene	$C_3H_8N_2$	3880-48-6		998
Methyl ethyl ether	C₃H₅O	540 <u>-</u> 67 <u>-</u> 0	Ethers	927
Methyl ethyl ketone	C₄H ₈ O	78-93-3	Ketones	938
2-Methyl-3-ethyl-1-pentene	C ₈ H ₁₆	19780-66-6	s-Alkenes	857
Methyl fluoride	CH₃F	593-53-3	Fluoride	1058
N-Methylformamide	C₂H₅NO	123-39-7	Amides	1008
Methyl formate	$C_2H_4O_2$	107–31–3	Esters	966
N-Methylglycine	C ₃ H ₇ NO ₂	107–97–1	Amino acids	1014
2-Methylheptane	C ₈ H ₁₈	592-27-8	t-Alkanes	836
3-Methylheptane	C_8H_{18}	111002-96-1	t-Alkanes	837
4-Methylheptane	C_8H_{18}	589–53–7	t-Alkanes	838
Methyl heptanoate	$C_8H_{16}O_2$	106730	Esters	967
Methyl hexadecanoate	$C_{17}H_{34}O_2$	112-39-0	Esters	968
2-Methylhexane	C ₇ H ₁₆	591–76–4	t-Alkanes	836
3-Methylhexane	C ₇ H ₁₆	589-34-4	t-Alkanes	837
Methyl hexanoate	$C_7H_{14}O_2$	106-70-7	Esters	966
3-Methyl-cis-3-hexene	C_7H_{14}	4914-89-0	s-Alkenes	853,854
3-Methyl-trans-3-hexene	C_7H_{14}	3899-36-3	s-Alkenes	851
Methyl hexyl ketone	$C_8H_{16}O$	111-13-7	Ketones	939
Methylhydrazine	CH ₆ N ₂	60-34-4	Hydrazines	997
Methyl iodide	CH ₃ I	74-88-4	Iodide	1092
Methyl 2-iodobenzoate	C ₈ H ₇ IO ₂	610–97–9	Iodide	1092
Methyl 3-iodobenzoate	C ₈ H ₇ IO ₂	618-91-7	Iodide	1098
Methyl 4-iodobenzoate	C ₈ H ₇ IO ₂	619-44-3	Iodide	1098
1-Methyl-2-isopropylbenzene	C ₁₀ H ₁₄	527-84-4	Aromat01	
1-Methyl-3-isopropylbenzene	C ₁₀ H ₁₄ C ₁₀ H ₁₄	535-77-3		869
1-Methyl-4-isopropylbenzene			Aromat01	869
	$C_{10}H_{14}$	99-87-6	Aromat01	869
Methyl isopropyl ether	C ₄ H ₁₀ O	598-53-8	Ethers	927,928
Methyl isopropyl ketone	C ₅ H ₁₀ O	563-80-4	Ketones	940
Methyl isovalerate	$C_6H_{12}O_2$	556-24-1	Esters	971
Methyl laurate	$C_{13}H_{26}O_2$	111-82-0	Esters	967
Methyl methacrylate	$C_5H_8O_2$	80-62-6	Esters	971
N-Methylmethanamide	C_2H_5NO	123–39–7	Amides	1008
Methyl methanoate	$C_2H_4O_2$	107_31_3	Esters	966
Methyl 2-methylbutanoate	$C_6H_{12}O_2$	868–57–5	Esters	970
Methyl 3-methylbutanoate	$C_6H_{12}O_2$	556–24–1	Esters	971
1-Methyl-4-(1-methylethenylsulfonyl)benzene	$C_{10}H_{12}O_2S$	67605-02-1	Sulfones	1053
Methyl 2-methylpropenoate	$C_5H_6O_2$	80626	Esters	971
1-Methyl-4-(2-methyl-2-propenylsulfonyl)benzene	$C_{11}H_{14}O_2S$	16192-04-4	Sulfones	1054
Methyl myristate	$C_{15}H_{30}O_2$	124-10-7	Esters	968
1-Methylnaphthalene	$C_{11}H_{10}$	90-12-0	Aromat02	879
2-Methylnaphthalene	$C_{11}H_{10}$	91-57-6	Aromat02	879,880
Methyl nitrate	CH ₃ NO ₃	598-58-3	Nitrates	•
Methyl nitrite	CH ₃ NO ₂			1032
mony muno		624–91–9	Nitrites	1031
1 Mathyl 2 nitrohanzana	$C \square N \cap$			
1-Methyl-2-nitrobenzene	C ₇ H ₇ NO ₂	88-72-2	Nitros	1026
1-Methyl-3-nitrobenzene	C ₇ H ₇ NO ₂	99-08-1	Nitros	1026

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
N-Methyl-N-nitro-(2,4,6-trinitro)aniline	C ₇ H ₅ N ₅ O ₈	479-45-8	Nitramines	1034
2-Methylnonane	$C_{10}H_{22}$	871–83–0	t-Alkanes	836
3-Methylnonane	$C_{10}H_{22}$	5911-04-6	t-Alkanes	837
4-Methylnonane	$C_{10}H_{22}$	17301–94–9	t-Alkanes	838
5-Methylnonane	$C_{10}H_{22}$	15869-85-9	t-Alkanes	838
Methyl nonanoate	$C_{10}H_{20}O_2$	1731-84-6	Esters	967
2-Methyloctane	C_9H_{20}	3221–61–2	t-Alkanes	836
3-Methyloctane	C_9H_{20}	2216-33-3	t-Alkanes	837
4-Methyloctane	C_9H_{20}	2216–34–4	t-Alkanes	838
Methyl octanoate	$C_9H_{18}O_2$	111–11–5	Esters	967
2-Methyloxirane	C₃H ₆ O	75–56–9	Ethers	933
Methyl palmitate	$C_{17}H_{34}O_2$	112-39-0	Esters	968
Methyl pentadecanoate	$C_{16}H_{32}O_2$	7132-64-1	Esters	968
Methyl pentadecylate	$C_{16}H_{32}O_2$	7132-64-1	Esters	968
N-Methylpentanamide	C ₆ H ₁₃ NO	6225-10-1	Amides	1009
Methyl pentanoate	$C_6H_{12}O_2$	624–24–8	Esters	966
2-Methylpentane	C_6H_{14}	107-83-5	t-Alkanes	835
3-Methylpentane	C_6H_{14}	96–14–0	t-Alkanes	837
2-Methyl-2-pentanethiol	$C_6H_{14}S$	1633–97–2	Thiols	1040
2-Methyl-3-pentanol	$C_6H_{14}O$	565673	Alcohols	916
4-Methyl-2-pentanol	$C_6H_{14}O$	108-11-2	Alcohols	916
2-Methyl-3-pentanone	$C_6H_{12}O$	565-69-5	Ketones	941
3-Methyl-1-pentene	C_6H_{12}	29564689	s-Alkenes	853
2-Methyl-1-pentene	C_6H_{12}	763-29-1	s-Alkenes	852
2-Methyl-2-pentene	C_6H_{12}	625-27-4	s-Alkenes	852
cis-3-Methyl-2-pentene	C_6H_{12}	922-61-2	s-Alkenes	853
trans-3-Methyl-2-pentene	C ₆ H ₁₂	616-12-6	s-Alkenes	853
4-Methyl-1-pentene	C ₆ H ₁₂	691–37–2	s-Alkenes	854
cis-4-Methyl-2-pentene	C ₆ H ₁₂	691–38–3	s-Alkenes	854
trans-4-Methyl-2-pentene	C ₆ H ₁₂	674-76-0	s-Alkenes	854
Methyl pentyl sulfide	C ₆ H ₁₄ S	1741-83-9	Sulfides	1043
Methyl perlargonate	$C_{10}H_{20}O_2$	1731-84-6	Esters	967
2-Methylphenol	C ₇ H ₈ O	95-48-7	Alcohols	921
3-Methylphenol	C ₇ H ₈ O	108-39-4	Alcohols	921
4-Methylphenol	C ₇ H ₈ O	106-44-5	Alcohols	921
3-Methylphenyl acetate	$C_9H_{10}O_2$	122-46-3	Esters	976
N-Methyl-N-phenylaniline	$C_{13}H_{13}N$	552-82-9	Amines	990
3-Methylphenyl ethanoate	$C_9H_{10}O_2$	122-46-3	Esters	976
Methyl phenyl ether	C ₇ H ₈ O	100-66-3	Ethers	934
1-Methyl-1-phenylethyl hydroperoxide	$C_9H_{12}O_2$	80–15–9	Hydroperoxides	980
Methyl phenyl ketone	C ₈ H ₈ O	98–86–2	Ketones	944
Methyl phenyl sulfide	C ₇ H ₈ S	100-68-5	Sulfides	1047
Methyl phenyl sulfone	C ₇ H ₈ O ₂ S	3112-85-4	Sulfones	1057
N-Methylpiperidine	C ₆ H ₁₃ N	626-67-5	CyclCHN	1003
2-Methylpiperidine	$C_6H_{13}N$	109057	CyclCHN	1003
4-Methylpiperidine	C ₆ H ₁₃ N	626-58-4	CyclCHN	1004
Methyl pivalate	C ₆ H ₁₂ O ₂	598-98-1	Esters	971
1-Methyl-4-(1,2-propadienylsulfonyl)benzene	$C_{10}H_{10}O_2S$	16192-08-8	Sulfones	1053
2-Methylpropanal	C ₁₀ H ₁₀ O ₂ S C ₄ H ₈ O	78-84-2		
7 1 1			Aldehyde	937
N-Methylpropanamide	C4H ₉ NO	1187–58–2	Amides	1009
2-Methylpropanamide	C₄H₀NO	563-83-7	Amides	1007
2-Methylpropane	C4H ₁₀	75–28–5	t-Alkanes	835
2-Methylpropanenitrile	C₄H ₇ N	78–82–0	Nitriles	994
2-Methyl-1-propanethiol	$C_4H_{10}S$	513-44-0	Thiols	1039
2-Methyl-2-propanethiol	C ₄ H ₁₀ S	75–66–1	Thiols	1039
Methyl propanoate	C ₄ H ₈ O ₂	554-12-1	Esters	966
2-Methyl-1-propanol	C ₄ H ₁₀ O	78–83–1	Alcohols	914
2-Methyl-2-propanol	C ₄ H ₁₀ O	75-65-0	Alcohols	у16,917
2-Methyl-1,2-propanediamine	$C_4H_{12}N_2$	811–93–8	Amines	985
2-Methyl-1,2-propanediol	$C_4H_{10}O_2$	558-43-0	Alcohols	918
2-Methylpropanoyl chloride	C ₄ H ₇ ClO	79–30–1	Chloride	1084
2-Methylpropene	C_4H_8	115–11–7	s-Alkenes	852
Methyl propenoate	$C_4H_6O_2$	96 33 3	Esters	971
1-Methyl-2-propenylbenzene	$C_{10}H_{12}$	934–10–1	Aromat02	874
1-Methyl-4-(2-propenylsulfonyl)benzene	$C_{10}H_{12}O_2S$	3112-87-6	Sulfones	1053

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
(E)-1-Methyl-4-(1-propenylsulfonyl)benzene	$C_{10}H_{12}O_2S$	32228-15-2	Sulfones	1053
N-Methylpropionamide	C ₄ H ₉ NO	1187–58–2	Amides	1009
Methyl propionate	C ₄ H ₈ O ₂	554-12-1	Esters	966
(2-Methyl)propoxy-2-(2-methyl)propane	C ₈ H ₁₈ O	6163-66-2	Ethers	929
2-Methylpropyl amine	C ₄ H ₁₁ N	78-81-9	Amines	983
(1-Methylpropyl)benzene	C ₁₀ H ₁₄	135-98-8	Aromat02	872
(2-Methylpropyl)benzene	C ₁₀ H ₁₄	538-93-2	Aromat02	873
1-Methyl-2-propylbenzene	C ₁₀ H ₁₄	1074–17–5	Aromat01	868
1-Methyl-3-propylbenzene	$C_{10}H_{14}$	1074-43-7	Aromat01	869
1-Methyl-4-propylbenzene	C ₁₀ H ₁₄	1074-55-1	Aromat01	869
2-Methylpropyl dichloroacetate	C ₆ H ₁₀ Cl ₂ O ₂	37079-08-6	Chloride	1083
N-(2-Methyl-2-propyl)ethanamide	C ₆ H ₁₃ NO	762-84-5	Amides	1009
2-Methylpropyl ethanoate	$C_6H_{12}O_2$	110-19-0	Esters	969
Methyl propyl ether	C ₄ H ₁₀ O C ₈ H ₁₇ N	557-17-5 6898-75-5	Ethers Imines	927
N-(2-Methylpropylidene)butylamine	$C_{5}H_{10}O$	107-87-9	Ketones	992
Methyl propyl ketone	$C_5H_{10}O_2$	542-55-2	Esters	938,939
2-Methylpropyl methanoate Methyl propyl sulfide	C ₅ H ₁₀ O ₂ C ₄ H ₁₀ S	3877-15-4	Sulfides	969
1-Methyl-4-(1-propynylsulfonyl)benzene	$C_{10}H_{10}O_2S$	14027–53–3	Sulfones	1042
1-Metnyl-4-(1-propynylsulfonyl)benzene	$C_{10}H_{10}O_2S$ $C_{10}H_{10}O_2S$	16192-07-7	Sulfones	1053
2-Methylpyridine	C ₁₀ 11 ₁₀ O ₂ 3 C ₆ H ₇ N	10192-07-7	CyclCHN	1053 1004
3-Methylpyridine	C ₆ H ₇ N	108-99-6	CyclCHN	1004
4-Methylpyridine	C ₆ H ₇ N	108-89-4	CyclCHN	1004
N-Methylpyrrole	C₅H₁N C₅H₁N	96–54–8	CyclCHN	1004
N-Methylpyrrolidine	C ₅ H ₁₁ N	120-94-5	CyclCHN	1002
meta -Methylstyrene	C ₂ H ₁₀	100-80-1	Aromat02	873
onho - Methylstyrene	C ₂ H ₁₀	611 15 4	Aromat02	873 873
para-Methylstyrene	C ₉ H ₁₀	622-97-9	Aromat02	873,874
α-Methylstyrene	C ₉ H ₁₀	98-83-9	Aromat02	874
cis-β-Methylstyrene	C ₉ H ₁₀	766–90–5	Aromat02	874
trans-β-Methylstyrene	C ₉ H ₁₀	873–66–5	Aromat02	874
Methylsuccinic acid	C ₅ H ₈ O ₄	498–21–5	Acids	954
Methylsuccinic anhydride	C₅H ₆ O₃	4100-80-5	Anhydrides	964
Methyl tetradecanoate	$C_{15}H_{30}O_2$	124-10-7	Esters	968
2-Methyl thiolane	C ₅ H ₁₀ S	1795-09-1	CyclCHS	1057
3-Methyl thiolane	$C_5H_{10}S$	4740-00-5	CyclCHS	1057
2-Methylthiophene	C₅H ₆ S	554-14-3	CyclCHS	1057
3-Methylthiophene	C5H6S	616-44-4	CyclCHS	1057
Methyl tolyl ether	$C^6H^{10}O$	100-84-5	Ethers	934
Methyl p-tolyl sulfone	$C_8H_{10}O_2S$	3185-99-7	Sulfones	1052
Methyl tridecanoate	$C_{14}H_{28}O_2$	1731–88–0	Esters	968
Methyl tridecylate	$C_{14}H_{28}O_2$	1731–88–0	Esters	968
Methyl <i>n</i> -tridecyl ketone	$C_{15}H_{30}O$	2345-28-0	Ketones	940
Methyl undecanoate	$C_{12}H_{24}O_2$	1731-86-8	Esters	967
Methyl undecylate	$C_{12}H_{24}O_2$	1731868	Esters	967
Methylurea	$C_2H_6N_2O$	598-50-5	Ureas	1011
Methyl valerate	$C_6H_{12}O_2$	624-24-8	Esters	966
Myristic acid	$C_{14}H_{28}O_2$	544638	Acids	948
Myristonitrile	$C_{14}H_{27}N$	629–63–0	Nitriles	994
N				
Naphthacene	C ₁₈ H ₁₂	92-24-0	Aromat02	885
Naphthalene	$C_{10}H_8$	91-20-3	Aromat02	878
1,2-Naphthalenediol	$C_{10}H_8O_2$	574-00-5	Alcohols	925
1,3-Naphthalenediol	$C_{10}H_8O_2$	132-86-5	Alcohols	925,926
1,4-Naphthalenediol	$C_{10}H_8O_2$	571608	Alcohols	926
2,3-Naphthalenediol	$C_{10}H_8O_2$	92-44-4	Alcohols	925
1-Naphthoic acid	$C_{11}H_8O_2$	86-55-5	Acids	962
2-Naphthoic acid	$C_{11}H_8O_2$	93-09-4	Acids	962,963
1-Naphthol	$C_{10}H_8O$	90–15–3	Alcohols	924
2-Naphthol	$C_{10}H_8O$	135–19–3	Alcohols	925
	0.11.11.0	60202 02 5	Ureas	1013
N'-(1-Naphthyl)-N,N-diphenylurea	$C_{23}H_{18}N_2O$	60302-02-5	Oreas	101.5
2-Nitroaniline	$C_6H_6N_2O_2$	88-74-4	Nitros	1028

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
Nitrobenzene	C ₆ H ₅ NO ₂	98-95-3	Nitros	102:
2-Nitrobenzoic acid	C7H5NO4	552-16-9	Nitros	1030
3-Nitrobenzoic acid	$C_7H_5NO_4$	121-92-6	Nitros	1030,103
4-Nitrobenzoic acid	$C_7H_5NO_4$	62-23-7	Nitros	103
1-Nitrobutane	$C_4H_9NO_2$	627-05-4	Nitros	102:
2-Nitrobutane	C ₄ H ₉ NO ₂	600–24–8	Nitros	1023,102
Nitroethane	C ₂ H ₅ NO ₂	79–24–3	Nitros	1025,102
Nitroglycerine	C ₃ H ₅ N ₃ O ₉	55-63-0	Nitrates	103:
Nitromethane	CH ₃ NO ₂	75–52–5	Nitros	1022
Nitromethylbenzene	$C_7H_7NO_2$	622-42-4	Nitros	1026,102
1-Nitronaphthalene	$C_{10}H_7NO_2$	86-57-7	Nitros	1020,102
1-Nitropentane	$C_{5}H_{11}NO_{2}$	628-05-7	Nitros	
		554–84–7		1023
m-Nitrophenol	C ₆ H ₅ NO ₃		Nitros	102
o-Nitrophenol	C ₆ H ₅ NO ₃	88–75–5	Nitros	102
p-Nitrophenol	C ₆ H ₅ NO ₃	100-02-7	Nitros	1027,102
2-Nitrophenol	C ₆ H ₅ NO ₃	88–75–5	Nitros	102
3-Nitrophenol	C ₆ H ₅ NO ₃	554-84-7	Nitros	102
4-Nitrophenol	$C_6H_5NO_3$	100-02-7	Nitros	1027,1028
N-Nitropiperidine	$C_5H_{10}N_2O_2$	7119-94-0	Nitramines	1034
1-Nitropropane	$C_3H_7NO_2$	108-03-2	Nitros	1023
2-Nitropropane	$C_3H_7NO_2$	79-46-9	Nitros	1023
Nitrosobenzene	C ₆ H ₅ NO	586-96-9	Nitroso	1021
4-Nitroso-1-naphthol	$C_{10}H_7NO_2$	605–60–7	Nitroso	1021
N-Nitrosopiperidine	$C_{5}H_{10}N_{2}O$	100-75-4	Nitroso	1021
• •		88-72-2		
2-Nitrotoluene	C ₇ H ₇ NO ₂		Nitros	1026
3-Nitrotoluene	C ₇ H ₇ NO ₂	99-08-1	Nitros	1026
4-Nitrotoluene	$C_7H_7NO_2$	99–99–0	Nitros	1026
Nitrourea	$CH_3N_3O_3$	556–89–8	Nitramines	1033
Nonadecane	$C_{19}H_{40}$	629–92–5	n-Alkanes	833
Nonadecanoic acid	$C_{19}H_{38}O_2$	646–30–0	Acids	949
Nonadecanol	$C_{19}H_{40}O$	1454–84–8	Alcohols	913
n-Nonadecyl alcohol	$C_{19}H_{40}O$	1454-84-8	Alcohols	913
Nonadecylic acid	$C_{19}H_{38}O_2$	646-30-0	Acids	949
Nonaldehyde	C ₂ H ₁₈ O	124-19-6	Aldehyde	937
Nonanal	C ₉ H ₁₈ O	124–19–6	Aldehyde	937
Nonane	C ₉ H ₂₀	111-84-2	•	
			n-Alkanes	831
Nonanedioic acid	C ₉ H ₁₆ O ₄	123–99–9	Acids	953
1-Nonanethiol	C ₉ H ₂₀ S	1455–21–6	Thiols	1037
Nonanoic acid	$C_9H_{18}O_2$	112-05-0	Acids	947
Nonanol	$C_9H_{20}O$	143-08-8	Alcohols	911
5-Nonanone	C ₉ H ₁₈ O	502–56–7	Ketones	939,940
1-Nonene	C_9H_{18}	124-11-8	n-Alkenes	847
n-Nonyl alcohol	$C_9H_{20}O$	143-08-8	Alcohols	911
Nonylbenzene	C ₁₅ H ₂₄	1081-77-2	Aromat01	867
Nonylcyclopentane	$C_{14}H_{28}$	2882-98-6	Cyclic02	894
1-Nonyne	C ₉ H ₁₆	3452-09-3	Alkynes	859
Norbornadiene	C ₇ H ₈	121-46-0	Cyclic03	902
Norbornane	C ₇ H ₁₂	279–23–2	Cyclic03	903
			•	
Norbornene	C ₇ H ₁₀	498–66–8	Cyclic03	903
Norleucine	$C_6H_{13}NO_2$	616–06–8	Amino acids	1016
0				
	_			
Octadecane	$C_{18}H_{38}$	593-45-3	n-Alkanes	833
Octadecanoic acid	$C_{18}H_{36}O_2$	57–11–4	Acids	949
Octadecanol	$C_{18}H_{38}O$	112-92-5	Alcohols	913
n-Octadecyl alcohol	$C_{18}H_{38}O$	112-92-5	Alcohols	913
1,7-Octadiyne	C ₈ H ₁₀	871–84–1	Alkynes	862
2,2,3,3,4,4,5,5-Octafluoro-1,6-hexanediol	$C_6H_6F_8O_2$	355-74-8	Fluoride	1064
Octafluoropropane	C_3F_8	76–19–7	Fluoride	1065
Octahydroazocine	C ₇ H ₁₅ N	1121-92-2	CyclCHN	1005
Octaldehyde	C ₆ H ₁₆ O	124-13-0	Aldehyde	937
Octanal	$C_8H_{16}O$	124–13–0	Aldehyde	937
Octanamide	$C_8H_{17}NO$	629–01–6	Amides	1008
Octane	C_8H_{18}	111-65-9	n-Alkanes	831

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
Octanenitrile	C ₈ H ₁₅ N	124-12-9	Nitriles	993
1-Octanethiol	$C_8H_{18}S$	111-88-6	Thiols	1036,1037
Octanoic acid	$C_8H_{16}O_2$	124-07-2	Acids	947
Octanol	$C_8H_{18}O$	111-87-5	Alcohols	911
2-Octanone	$C_8H_{16}O$	111–13–7	Ketones	939
1-Octene	C_8H_{16}	111660	n-Alkenes	847
cis-2-Octene	C_8H_{16}	7642-04-8	n-Alkenes	849
trans-2-Octene	C_8H_{16}	13389-42-9	n-Alkenes	849
1-Octen-3-yne	C_8H_{12}	17679-92-4	Alkynes	861
Octogen	$C_4H_8N_8O_8$	2691-41-0	Nitramines	1034
n-Octyl alcohol	$C_8H_{18}O$	111-87-5	Alcohols	911
Octylbenzene	$C_{14}H_{22}$	2189-60-8	Aromat01	867
Octylcyclopentane	$C_{13}H_{26}$	1795-20-6	Cyclic02	894
1-Octyne	C ₈ H ₁₄	629-05-0	Alkynes	859
DL-Ornithine	$C_5H_{12}N_2O_2$	616-07-9	Amino acids	1017
Oxalic acid	$C_2H_2O_4$	144-62-7	Acids	
				951
Oxane	C ₅ H ₁₀ O	142687	Ethers	934
Oxetane	C₃H ₆ O	503300	Ethers	933
2-Oxetanone	C ₃ H ₄ O ₂	57–57–8	Esters	975
Oxirane	C₂H₄O	75–21–8	Ethers	932
Oxolane	C_4H_8O	109999	Ethers	933
1,1'-Oxybisbenzene	$C_{12}H_{10}O$	101-84-8	Ethers	935
1,1'-Oxybisethene	C₄H ₆ O	109-93-3	Ethers	929
P				
Palmitic acid	$C_{16}H_{32}O_2$	57-10-3	Acids	948,949
2,2-Paracyclophane	$C_{16}H_{16}$	1633223	Cyclic02	901
3,3-Paracyclophane	$C_{18}H_{20}$	2913-24-8	Cyclic02	901
Pelargonic acid	$C_9H_{18}O_2$	112-05-0	Acids	947
Pentachlorobenzene	C ₆ HCl ₅	608-93-5	Chloride	1075,1076
Pentachloroethane	C ₂ HCl ₅	76-01-7	Chloride	1070
Pentachlorophenol	C₀HCl₅O	87-86-5	Chloride	1078
Pentacosane	$C_{25}H_{52}$	629-99-2	n-Alkanes	834
Pentacyclo[4.2.0.0 ² ,5.0 ³ ,8.0 ⁴ ,7]octane	C ₈ H ₈	277-10-1	Cyclic03	904
Pentadecane	$C_{15}H_{32}$	629-62-9	n-Alkanes	832
Pentadecanoic acid	$C_{15}H_{30}O_2$	1002-84-2	Acids	
Pentadecanol	C ₁₅ H ₃₂ O	629-76-5		948
			Alcohols	912
2-Pentadecanone	$C_{15}H_{30}O$	2345–28–0	Ketones	940
n-Pentadecyl alcohol	$C_{15}H_{32}O$	629-76-5	Alcohols	912
Pentadecylic acid	$C_{15}H_{30}O_2$	1002–84–2	Acids	948
1,2-Pentadiene	C ₅ H ₈	591–95–7	n-Alkenes	850
cis-1,3-Pentadiene	C_5H_8	1574-41-0	n-Alkenes	850
trans-1,3-Pentadiene	C_5H_8	2004–70–8	n-Alkenes	851
1,4-Pentadiene	C_5H_8	591–93–5	n-Alkenes	851
2,3-Pentadiene	C_5H_8	591–96–8	n-Alkenes	851
Pentaerythritol	$C_5H_{12}O_4$	115 –77– 5	Alcohols	919
Pentaethylbenzene	$C_{16}H_{26}$	605-01-6	Aromat02	872
Pentafluorobenzene	C ₆ HF ₅	363-72-4	Fluoride	1062,1063
Pentafluorobenzoic acid	C7HF5O2	602–94–8	Fluoride	1064
Pentafluorophenol	C₄HF₅O	771-61-9	Fluoride	1064
2,2,3,3,3-Pentafluoro-1-propanol	C ₃ H ₃ F ₅ O	422-05-9	Fluoride	
2,3,4,5,6-Pentafluorotoluene	C ₇ H ₃ F ₅			1064
		771–56–2	Fluoride	1063
Pentafluoro(trifluoromethyl)benzene	C_7F_8	434-64-0	Fluoride	1060
Pentaldehyde	C ₁ H ₁₀ O	110–62–3	Aldehyde	936
Pentamethyl benzoic acid	$C_{12}H_{16}O_2$	2243–32–5	Acids	961
Pentamethylbenzene	$C_{11}H_{16}$	700–12–9	Aromat01	865
Pentanal	$C_5H_{10}O$	110-62-3	Aldehyde	936
Pentanamide	C ₅ H ₁₁ NO	626-97-1	Amides	1007
Pentane	C_5H_{12}	109660	n-Alkanes	830
1,5-Pentanedinitrile	$C_5H_6N_2$	544-13-8	Nitriles	996
Pentanedioic acid	C₅H ₈ O ₄	110-94-1	Acids	952
1,5-Pentanediol	C ₅ H ₁₂ O ₂	111-29-5	Alcohols	919
2,4-Pentanedione	C ₅ H ₈ O ₂	123-54-6	Ketones	942
1,5-Pentanedithiol	$C_5H_{12}S_2$	928-98-3	Thiols	1038
		240 70- .1	LIHOIS	10.58
Pentanenitrile	C ₅ H ₉ N	110-59-8	Nitriles	993

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
1-Pentanethiol	C₅H₁2S	110–66–7	Thiols	1036
Pentanoic acid	$C_5H_{10}O_2$	109-52-4	Acids	946
Pentanol	C ₅ H ₁₂ O	71-41-0	Alcohols	910
2-Pentanol	C₅H ₁₂ O	6032–29–7	Alcohols	915
3-Pentanol	C ₅ H ₁₂ O	584-02-1	Alcohols	915
4-Pentanolactone	$C_5H_8O_2$	108-29-2	Esters	975
5-Pentanolactone	$C_5H_8O_2$	542-28-9	Esters	975
2-Pentanone	$C_5H_{10}O$	107–87–9	Ketones	938,939
3-Pentanone	C ₅ H ₁₀ O	96–22–0	Ketones	939
Pentanoyl chloride	C₅H₀ClO	638–29–9	Chloride	1084
Pentaphenylethane	C ₃₂ H ₂₆	19112–42–6	Aromat02	877
1-Pentene	C ₅ H ₁₀	109-67-1	n-Alkenes	846
cis-2-Pentene	C₅H ₁₀	627–20–3	n-Alkenes	848
trans-2-Pentene	C ₅ H ₁₀	646-04-8	n-Alkenes	848
trans-2-Pentenenitrile	C ₅ H ₇ N	26294-98-4	Nitriles	995
trans-3-Pentenenitrile	C ₅ H ₇ N	16529-66-1	Nitriles	995
cis-3-Penten-1-yne	C₅H ₆	1574-40-9	Alkynes	861
trans-3-Penten-1-yne	C₅H ₆	2004–69–5	Alkynes	861
2,2,3,4,4-Pentmethylpentane	$C_{10}H_{22}$	16747-45-8	q-Alkanes	845
n-Pentyl alcohol	C ₅ H ₁₂ O	71-41-0	Alcohols	910
n-Pentyl amine	C ₅ H ₁₃ N	110–58–7	Amines	983
Pentylbenzene	C11H16	700_12_9	Aromat01	866
Pentylcyclohexane	$C_{11}H_{22}$	4292–92–6	Cyclic02	898
Pentylcyclopentane	$C_{10}H_{20}$	3741-00-2	Cyclic02	893
1-Pentylnaphthalene	$C_{15}H_{18}$	86–89–5	Aromat02	881
2-Pentylnaphthalene	C ₁₅ H ₁₈	93-22-1	Aromat02	881
1-Pentyne	C ₅ H ₈	627-19-0	Alkynes	858,859
2-Pentyne	C_5H_8	627–21–4	Alkynes	860
Perbenzoic acid	$C_7H_6O_3$	93-59-4	Peroxyacids	980
Perdodecanoic acid	$C_{12}H_{24}O_3$	2388-12-7	Peroxyacids	980
Perfluoropropane	C ₃ F ₈	76–19–7	Fluorides	1065
Perhexadecanoic acid	$C_{16}H_{32}O_3$	7311–29–7	Peroxyacids	981
Peroctadecanoic acid	$C_{18}H_{36}O_3$	5796–86–1	Peroxyacids	981
Peroxylauric acid	$C_{12}H_{24}O_3$	2388–12–7	Peroxyacids	980
Peroxymyristic acid	$C_{14}H_{28}O_3$	19816-73-0	Peroxyacids	980
Peroxypalmitic acid	$C_{16}H_{32}O_3$	7311–29–7	Peroxyacids	981
Peroxystearic acid	$C_{18}H_{36}O_3$	5796–86–1	Peroxyacids	981
Pertetradecanoic acid	$C_{14}H_{28}O_3$	19816730	Peroxyacids	980
Perylene	$C_{20}H_{12}$	198–55–0	Aromat02	886
Phenanthrene	$C_{14}H_{10}$	85-01-8	Aromat02	885
Phenetole	$C_8H_{10}O$	103-73-1	Ethers	934
Phenol	C ₆ H ₆ O	108-95-2	Alcohols	921
N-Phenylacetamide	C ₈ H ₉ NO	103-84-4	Amides	1010
Phenyl acetate	$C_8H_8O_2$	122–79–2	Esters	976
DL-Phenylalanine	$C_9H_{11}NO_2$	150–30–1	Amino acids	1018
N-Phenylaniline	$C_{12}H_{11}N$	122-39-4	Amines	990
Phenylazide	$C_6H_5N_3$	622–37–7	Azides	1000
Phenyl benzoate	$C_{13}H_{10}O_2$	93-99-2	Esters	976
Phenylbutanedioic acid	$C_{10}H_{10}O_4$	635-51-8	Acids	963
1-Phenyl-1-butanone	$C_{10}H_{12}O$	495-40-9	Ketones	944
Phenylcarbinol	C_7H_8O	100–51–6	Alcohols	914
Phenylcyclopropane	C ₉ H ₁₀	873-49-4	Cyclic03	906
N-Phenylethanamide	C ₈ H ₉ NO	103-84-4	Amides	1010
Phenyl ethanoate	$C_8H_8O_2$	122-79-2	Esters	976
2-Phenylethylamine	$C_8H_{11}N$	64040	Amines	990
N-Phenylglycine	$C_8H_9NO_2$	103-01-5	Amino acids	1019
Phenylhydrazine	$C_6H_8N_2$	100-63-0	Hydrazines	998
N-(Phenylmethylene)benzenimine	$C_{13}H_{11}N$	538-51-2	Imines	992
Phenylnitromethane	$C_7H_7NO_2$	622-42-4	Nitros	1026,1027
1-Phenyl-1-propanone	$C_9H_{10}O$	93-55-0	Ketones	944
1-Phenyl-2-propanone	$C_9H_{10}O$	103-79-7	Ketones	944
trans-Phenyl β-styryl sulfone	$C_{14}H_{12}O_2S$	16212069	Sulfones	1054
Phenylsuccinic acid	$C_{10}H_{10}O_4$	635-51-8	Acids	963
Phenyl p-tolyl ketone	C ₁₄ H ₁₂ O	134-84-9	Ketones	944
Phenylurea	C ₇ H ₈ N ₂ O	64–10–8	Ureas	1013
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TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
Phthalic acid	C ₈ H ₆ O ₄	88-99-3	Acids	961
Phthalic anhydride	$C_8H_4O_3$	85-44-9	Anhydrides	965
1,2-Phthaloyl chloride	$C_8H_4Cl_2O_2$	88-95-9	Chloride	1085
1,3-Phthaloyl chloride	C ₈ H ₄ Cl ₂ O ₂	100-20-9	Chloride	1085
1.4-Phthaloyl chloride	C ₈ H ₄ Cl ₂ O ₂	99638	Chloride	1085
2-Picoline	C_6H_7N	109068	CyclCHN	1004
3-Picoline	C_6H_7N	108-99-6	CyclCHN	1004
4-Picoline	C₀H ₇ N	108-89-4	CyclCHN	1004
Picramide	C ₆ H ₄ N ₄ O ₆	489–98–5	Nitros	1030
Picric acid	C ₆ H ₃ N ₃ O ₇	29663-11-4	Nitros	1028
Pimelic acid	C ₇ H ₁₂ O ₄	111-16-0	Acids	952
Piperidine	C ₃ H ₁₂ O ₄ C ₃ H ₁₁ N	110-89-4		
2			CyclCHN	1002
Pivalic acid	$C_5H_{10}O_2$	75-98-9	Acids	950
Pivalic anhydride	C ₁₀ H ₁₈ O ₃	1538-75-6	Anhydrides	964
Propanal	C₃H₄O	123-38-6	Aldehyde	935,936
Propanamide	C ₃ H ₇ NO	79050	Amides	1006,1007
Propane	C_3H_8	74-98-6	n-Alkanes	830
Propanediamide	$C_3H_6N_2O_2$	108-13-4	Amides	1010
1,2-Propanediamine	$C_3H_{10}N_2$	78-90-0	Amines	984
Propanedioic acid	$C_3H_4O_4$	141-82-2	Acids	951
1,2-Propanediol	$C_3H_8O_2$	57–55–6	Alcohols	917
1,3-Propanediol	C ₂ H ₈ O ₂	504-63-2	Alcohols	917
1,3-Propanedithiol	C ₃ H ₈ S ₂	109-80-8	Thiols	1038
Propanenitrile	C_3H_5N	107-12-0	Nitriles	992
•	C ₃ H ₈ S			
1-Propanethiol		107-03-1	Thiols	1035,1036
2-Propanethiol	C₃H ₈ S	75–33–2	Thiols	1038
1,2,3-Propanetriol	$C_3H_8O_3$	56-81-5	Alcohols	918
Propanoic acid	$C_3H_6O_2$	79094	Acids	945
Propanoic anhydride	$C_6H_{10}O_3$	123-62-6	Anhydrides	964
Propanol	C₃H ₈ O	71–23–8	Alcohols	910
2-Propanol	C₃H ₈ O	67630	Alcohols	915
3-Propanolactone	$C_3H_4O_2$	57-57-8	Esters	975
Propanone	C₃H₄O	67-64-1	Ketones	938
Propanoyl chloride	C₃H₅ClO	79-03-8	Chloride	1084
Proponenitrile	C ₃ H ₃ N	107-13-1	Nitriles	994
2-Propenoic acid	$C_3H_4O_2$	79-10-7	Acids	950
2-Propenol	C ₃ H ₆ O	107–18–6	Alcohols	
2-Propenylbenzene	C₀H₁0	300-57-2		909,910
cis-1-Propenylbenzene			Aromat02	874
	C ₂ H ₁₀	766–90–5	Aromat02	874
rans-1-Propenylbenzene	C ₉ H ₁₀	873–66–5	Aromat02	874
B-Propiolactone	C ₃ H ₄ O ₂	57-57-8	Esters	975
Propionaldehyde	C_3H_6O	123-38-6	Aldehyde	935,936
Propionamide	C₃H ₇ NO	79050	Amides	1006,1007
Propionic acid	$C_3H_6O_2$	79094	Acids	945
Propionic anhydride	$C_6H_{10}O_3$	123-62-6	Anhydrides	964
Propionitrile	C ₃ H ₅ N	107-12-0	Nitriles	992
2-Propoxyethanol	$C_5H_{12}O_2$	2807-30-9	Ethers	932
2-Propoxy-2-(2-methyl)propane	C ₇ H ₁₆ O	17348-59-3	Ethers	929
Ргорохургорапе	$C_6H_{14}O$	111-43-3	Ethers	
2-Propoxy-2-propane	C6H14O			926
		108-20-3	Ethers	928
V-Propylacetamide	C ₅ H ₁₁ NO	5331-48-6	Amides	1008
Propyl acctate	C ₅ H ₁₀ O ₂	109-60-4	Esters	969
-Propyl alcohol	C₃H ₈ O	71–23–8	Alcohols	910
-Propyl amine	C ₃ H ₉ N	107-10-8	Amines	982,983
Propylbenzene	C_9H_{12}	103-65-1	Aromat01	866
Propyl (E)-2-butenoate	$C_7H_{12}O_2$	10352-87-1	Esters	973
Propyl trans-2-butenoate	$C_7H_{12}O_2$	10352-87-1	Esters	973
Propyl chloroacetate	C ₅ H ₉ ClO ₂	5396-24-7	Chloride	1081
Propyl 2-chlorobutanoate	C ₇ H ₁₃ ClO ₂	62108-71-8	Chloride	1082
Propyl 4-chlorobutanoate	C ₇ H ₁₃ ClO ₂ C ₇ H ₁₃ ClO ₂	3153-35-3	Chloride	
Propyl 3-chloropropanoate	C ₆ H ₁₁ ClO ₂			1082
Propylcyclohexane		1487-41-8	Chloride	1082
	C ₂ H ₁₈	1678-92-8	Cyclic02	898
Propylcyclopentane	C_8H_{16}	2040-96-2	Cyclic01	893
Propylene	C₃H ₆	115-07-1	n-Alkenes	846
Propylene glycol Propylene oxide	$C_3H_8O_2$	57-55-6	Alcohols	917

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TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
N-Propylethanamide	C₅H ₁₁ NO	5331–48–6	Amides	100
N-2-Propylethanamide	C ₅ H ₁₁ NO	1118-69-0	Amides	100
Propyl ethanoate	$C_5H_{10}O_2$	109-60-4	Esters	969
4-Propylheptane	$C_{10}H_{22}$	3178-29-8	t-Alkanes	840
1-Propylnaphthalene	$C_{13}H_{14}$	2765-18-6	Aromat02	886
2-Propylnaphthalene	$C_{13}H_{14}$	2027–19–2	Aromat02	880
Propyl 2-pentenoate	$C_8H_{14}O_2$	62030-39-1	Esters	973,974
Propyl 3-pentenoate	$C_8H_{14}O_2$	62030-40-4	Esters	974
N-Propylpiperidine	$C_8H_{17}N$	5470-02-0	CyclCHN	1005,1006
n-Propyl nitrate	C ₃ H ₇ NO ₃	627-13-4	Nitrates	1032
n-Propyl nitrite	C ₃ H ₇ NO ₂	543-67-9	Nitrites	1031
Propyl pentanoate	$C_8H_{16}O_2$	141–06–0	Esters	970
** *				
Propyl phenyl ketone	$C_{10}H_{12}O$	495–40–9	Ketones	944
Propyl valerate	$C_8H_{16}O_2$	141-06-0	Esters	970
Propyne	C_3H_4	74997	Alkynes	858
1-(Propynylsulfonyl)benzene	C ₉ H ₈ O ₂ S	2525-41-9	Sulfones	1052
2-(Propynylsulfonyl)benzene	C ₉ H ₈ O ₂ S	2525408	Sulfones	1052
Pyrazine	$C_4H_4N_2$	290–37–9		
			CyclCHN	1003
Pyrene	$C_{16}H_{10}$	129-00-0	Aromat02	885
Pyridazine	$C_4H_4N_2$	289–80–5	CyclCHN	1002
Pyridine	C ₅ H ₅ N	110-86-1	CyclCHN	1001,1002
Pyrimidine	$C_4H_4N_2$	289-95-2	CyclCHN	1003
Pyrrole	C ₄ H ₅ N	109-97-7	CyclCHN	1003
Pyrrolidine	C ₄ H ₉ N	123–75–1		
•			CyclCHN	1001
Pyrrolizidine	$C_7H_{13}N$	643–20–9	CyclCHN	1006
Q				
Quadricyclane	C_7H_8	278-06-8	Cyclic03	903
Quinoline	C ₉ H ₇ N	91–22–5	CyclCHN	1003
R				
RDX	$C_3H_6N_6O_6$	121–82–4	Nitramines	1034
Resorcinol	$C_6H_6O_2$	108-46-3	Alcohols	924
R-salt	$C_3H_6N_6O_3$	13980-04-6	Nitroso	1022
S				
Salicylic acid	$C_7H_6O_3$	69–72–7	Acids	961
Sarcosine	$C_3H_7NO_2$	107-97-1	Amino acids	1014
Sebacic acid	$C_{10}H_{18}O_{4}$	111–20–6	Acids	953
DL-Serine	C ₃ H ₇ NO ₃	302-84-1	Amino acids	1017
		157-40-4		
Spiropentane	C₅H ₈		Cyclic01	890,891
Stearic acid	$C_{18}H_{36}O_2$	57–11–4	Acids	949
cis-Stilbene	$C_{14}H_{12}$	645_49_8	Aromat02	876
trans-Stilbene	$C_{14}H_{12}$	103300	Aromat02	876
Styrene	C_8H_8	100-42-5	Aromat02	873
cis-β-Styryl p-tolyl sulfone	$C_{15}H_{14}O_2S$	54897-33-5	Sulfones	1054
trans-β-Styryl p-tolyl sulfone	C ₁₅ H ₁₄ O ₂ S	16212-08-1	Sulfones	1054
Suberic acid	$C_8H_{14}O_4$	505-48-6	Acids	952
Succinamide	$C_4H_8N_2O_2$	110–14–5	Amides	1010
Succinic acid	$C_4H_6O_4$	110-15-6	Acids	951
Succinic anhydride	C ₄ H ₄ O ₃	108–30–5	Anhydrides	964
Succinimide				
	C ₄ H ₅ NO ₂	123-56-8	CyclCHNO	1035
Succinonitrile	C ₄ H ₄ N ₂	110–61–2	Nitriles	996
T				
Terephthalic acid	C ₈ H ₆ O ₄	100-21-0	Acids	962
•	$C_{18}H_{14}$	84-15-1	Aromat02	879
ortho-Terphenyl	C181 114			
ortho-Terphenyl		87–87–6	Chloride	1078
ortho-Terphenyl 2,3,5,6-Tetrachloro-1,4-benzenediol	$C_6H_2Cl_4O_2$			
ortho-Terphenyl 2,3,5,6-Tetrachloro-1,4-benzenediol 1,2,4,5-Tetrachloro-3,6-dimethylbenzene	$C_6H_2Cl_4O_2$ $C_8H_6Cl_4$	877–10–1	Chloride	1075
ortho-Terphenyl 2,3,5,6-Tetrachloro-1,4-benzenediol 1,2,4,5-Tetrachloro-3,6-dimethylbenzene 1,1,2,2-Tetrachloroethane	C ₆ H ₂ Cl ₄ O ₂ C ₈ H ₆ Cl ₄ C ₂ H ₂ Cl ₄	877-10-1 79-34-5	Chloride Chloride	1075 1070
ortho-Terphenyl 2,3,5,6-Tetrachloro-1,4-benzenediol 1,2,4,5-Tetrachloro-3,6-dimethylbenzene	$C_6H_2Cl_4O_2$ $C_8H_6Cl_4$	877–10–1	Chloride	1075

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
1,2,2,3-Tetrachioropropane	C ₃ H ₄ Cl ₄	13116–53–5	Chloride	1070
Tetracosane	$C_{24}H_{50}$	646-31-1	n-Alkanes	834
Tetracyclo[3.2.0 ^{2,7} .0 ^{4,6}]heptane	C_7H_8	278-06-8	Cyclic03	903
Tetradecane	C ₁₄ H ₃₀	629–59–4	n-Alkanes	832
Tetradecanenitrile	C ₁₄ H ₂₇ N	629-63-0	Nitriles	994
Tetradecanoic acid	$C_{14}H_{28}O_2$	544-63-8	Acids	948
Tetradecanol	C14H30O	112-72-1	Alcohols	912
2-Tetradecanone	C ₁₄ H ₂₈ O	2345-27-9	Ketones	940
n-Tetradecyl alcohol	C ₁₄ H ₃₀ O	112-72-1	Alcohols	912
Tetraethylbutanedioic acid	$C_{12}H_{22}O_4$	4111-60-8	Acids	956
Tetraethyleneglycol	$C_8H_{18}O_5$ $C_{12}H_{22}O_4$	112-60-7 4111-60-8	Ethers Acids	932
Tetraethylsuccinic acid	$C_{12}H_{22}O_4$ $C_9H_{20}N_2O$	1187-03-7	Ureas	956
Tetraethylurea	C ₆ H ₂ F ₄	2367–82–0	Fluoride	1012
1,2,3,5-Tetrafluorobenzene	C ₆ H ₂ F ₄	2307-82-0 327-54-8	Fluoride	1062
1,2,4,5-Tetrafluorobenzene 1,2,3,4-Tetrafluorobenzene	C ₆ H ₂ F ₄ C ₆ H ₂ F ₄	551-62-2	Fluoride	1062
	C ₂ F ₄	116-14-3	Fluoride	1062
Tetrafluoroethylene	C₂F4 C₃H4F4O	76-37-9	Fluoride	1059 1064
2,2,3,3-Tetrafluoro-1-propanol	C₃H₄P₄O C₄H ₈ O	109-99-9	Ethers	933
Tetrahydronyran	C ₅ H ₁₀ O	142-68-7	Ethers	933
Tetrahydropyran 3,4,5,6-Tetrahydro-3,3,6,6-tetramethylpyridazine	$C_8H_{16}N_2$	19403248	Diazene	934
Tetralite	$C_7H_5N_5O_8$	479-45-8	Nitramines	1034
Tetramethoxymethane	C ₃ H ₁₂ O ₄	1850-14-2	Ethers	930
1,2,3,4-tetramethylbenzene	C ₁₀ H ₁₄	488-23-3	Aromat01	864
1,2,3,5-Tetramethylbenzene	$C_{10}H_{14}$	527-53-7	Aromat01	864,865
1,2,4,5-Tetramethylbenzene	C ₁₀ H ₁₄	95–93–2	Aromat01	865
2,3,4,5-Tetramethyl benzoic acid	$C_{11}H_{14}O_2$	2408-38-0	Acids	960
2,3,4,6-Tetramethyl benzoic acid	$C_{11}H_{14}O_2$	2604–45–7	Acids	960,961
2,3,5,6-Tetramethyl benzoic acid	$C_{11}H_{14}O_2$	3854-90-8	Acids	961
2,2,3,3-Tetramethylbutane	C ₈ H ₁₈	594-82-1	g-Alkanes	844
Tetramethylbutanedioic acid	C ₈ H ₁₄ O ₄	630-51-3	Acids	955
1,1,4,4-Tetramethylcyclotetramethylenediazene	$C_8H_{16}N_2$	19403-24-8	Diazene	999
1,1,3,3-Tetramethylcyclotrimethylenediazene	$C_7H_{14}N_2$	2721-31-5	Diazene	999
2,2',5,5'-Tetramethyl-N,N-dipyrryl	$C_{12}H_{16}N_2$	10507-71-8	CyclCHN	1002
2,2,7,7-Tetramethylocta-3,5-diyne	$C_{12}H_{18}$	6130-98-9	Alkynes	862
2,2,6,6-Tetramethyl-4-heptanone	$C_{11}H_{22}O$	4436-99-1	Ketones	942
3,3,6,6,-Tetramethylocta-1,7-diyne	$C_{12}H_{18}$	64020560	Alkynes	862
Tetramethyl orthocarbonate	$C_5H_{12}O_2$	1850-14-2	Ethers	930
2,2,3,3-Tetramethylpentane	C_9H_{20}	7154–79–2	q-Alkanes	844,845
2,2,4,4-Tetramethylpentane	C ₉ H ₂₀	1070-87-7	q-Alkanes	845
2,2,4,4-Tetramethyl-3-pentanone	$C_9H_{18}O$	815–24–7	Ketones	941
3,3,5,5-Tetramethyl-1-pyrazoline	$C_7H_{14}N_2$	2721-31-5	Diazene	999
Tetramethylsuccinic acid	C _R H ₁₄ O ₄	630–51–3	Acids	955
Tetramethylsuccinic anhydride	C ₈ H ₁₂ O ₃	35046685	Anhydrides	965
Tetramethylurea	$C_5H_{12}N_2O$	632–22–4	Ureas	1011
Tetranitromethane	CN₄O ₈	509-14-8	Nitros	1022,1023
3,5,7,9-Tetraoxaundecane	C ₇ H ₁₆ O ₄	4431–82–7	Ethers	931
1,1,4,4-Tetraphenylbutane	C ₂₈ H ₂₆	1483-64-3	Cyclic03	908
1,1,1,2-Tetraphenylethane	$C_{26}H_{22}$	2294-94-2	Aromat02	877
1,1,2,2-Tetraphenylethane	$C_{26}H_{22}$	632–50–8	Aromat02	877
Tetraphenylethylene	$C_{26}H_{20}$	632-51-9	Aromat02	884
Tetraphenylmethane	C ₂₅ H ₂₀	630-76-2	Aromat02	876
Tetraphenylurea	C ₂₅ H ₂₀ N ₂ O	632–89–3	Ureas	1014
Tetryl	C ₇ H ₅ N ₅ O ₈	479-45-8	Nitramines	1034
Thiacyclobutane	C₃H₄S	287-27-4	CyclCHS	1056
Thiacycloheptane	C ₆ H ₁₂ S	4753-80-4	CyclCHS	1056
Thiacyclohexane Thiacyclonexane	C₅H₁₀S	1613-51-0	CyclCHS	1056
Thiacyclopentane Thiacyclopentane	C ₄ H ₈ S	110-01-0	CyclCHS	1056
Thiacyclopropane	C₂H₄S C₂H₄S	420–12–2 5206–62–8	CyclCHS	1056
4-Thia-1-hexene	C ₅ H ₁₀ S	5296-62-8	Sulfides	1046
Thiophene	C4H4S	110-02-1	CyclCHS	1057
DL-Threonine	C₄H ₉ NO ₃	80–68–2	Amino acids	1017
Toluene	C ₇ H ₈	108-88-3	Aromat01	863
p-Tolyl vinyl sulfone	C ₉ H ₁₀ O ₂ S	5535-52-4	Sulfones	1053
1,3,5-Triazine	C ₃ H ₃ N ₃	290-87-9	CyclCHN	1002
Tribenzylamine	$C_{21}H_{21}N$	620-40-6	Amines	988

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TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page
1,2,3-Tribromopropane	C ₃ H ₅ Br ₃	96–11–7	Bromide	1090
Γri-n-butylamine	$C_{12}H_{27}N$	102-82-9	Amines	98'
2,3,5-Trichloro-1,4-benzenediol	$C_6H_3Cl_3O_2$	608-94-6	Chloride	1078
2,2,3-Trichlorobutanal	C ₄ H ₅ Cl ₃ O	76–36–8	Chloride	1081
1,1,1-Trichloroethane	$C_2H_3Cl_3$	71-55-6	Chloride	1069
1,1,2-Trichloroethane	C ₂ H ₃ Cl ₃	79-00 5	Chloride	1069
Trichloroethylene	C₂HCl₃	79–01–6	Chloride	1072
1,2,3-Trichloropropane	C ₃ H ₅ Cl ₃	96-18-4	Chloride	1070
1,2,3-Trichloropropene	C ₃ H ₃ Cl ₃	96–19–5	Chloride	1072
1,3,5-Trichloro-2,4,6-trifluorobenzene	$C_6Cl_3F_3$	319–88–0	Mixed	1101
1,1,1-Trichloro-3,3,3-trifluoropropane	$C_3H_2Cl_3F_3$	7125–83–9	Mixed	1100
1,1,2-Trichloro-1,2,2-trifluoroethane	$C_2Cl_3F_3$	76–13–1	Mixed	1099,1100
Tricyclo[2.2.1.0 ^{2,6}]heptane	C_7H_{10}	279–19–6	Cyclic03	903
Tricyclo[3.3.1.1 ^{3,7}]dccanc	$C_{10}H_{16}$	281-23-2	Cyclic02	901
Tricyclo[3.3.1.1 ^{3,7}]decane-1-carboxamide	$C_{11}H_{17}NO$	5511–18–2	Amides	1010
Tridecane	$C_{13}H_{28}$	629–50–5	n-Alkanes	832
Tridecanedioic acid	$C_{13}H_{24}O_4$	505-52-2	Acids	954
Tridecanoic acid	$C_{13}H_{26}O_2$	638-53-9	Acids	948
Tridecanol	$C_{13}H_{28}O$	112 –7 0–9	Alcohols	912
n-Tridecyl alcohol	$C_{13}H_{28}O$	112-70-9	Alcohols	912
Tri-n-decylamine	$C_{30}H_{63}N$	1070-01-5	Amines	988
Tridecylic acid	$C_{13}H_{26}O_2$	638-53-9	Acids	948
Triethylamine	$C_6H_{15}N$	121-44-8	Amines	986,987
1,2,3-Triethylbenzene	$C_{12}H_{18}$	42205-08-3	Aromat02	871
1,2,4-Triethylbenzene	$C_{12}H_{18}$	877-44-1	Aromat02	871
1,3,5-Triethylbenzene	$C_{12}H_{18}$	102-25-0	Aromat02	871,872
Triethylbutanedioic acid	$C_{10}H_{18}O_4$	2103-18-6	Acids	956
Triethyleneglycol	$C_6H_{14}O_4$	112-27-6	Ethers	932
Triethylsuccinic acid	$C_{10}H_{18}O_4$	2103-18-6	Acids	956
1,1,1-Trifluorocthane	$C_2H_3F_3$	420-46-2	Fluoride	1059
1,1,2-Trifluoroethane	$C_2H_3F_3$	430-66-0	Fluoride	1059
2,2,2-Trifluoroethanol	C ₂ H ₃ F ₃ O	75–89–8	Fluoride	1063
Trifluoroethylene	C_2HF_3	359-11-5	Fluoride	1060
1,1,1-Trifluoro-2-iodoethane	$C_2H_2F_3I$	353-83-3	Mixed	1099
(Trifluoromethyl)benzene	$C_7H_5F_3$	98-08-8	Fluoride	1062
3,3,3-Trifluoro-1-propanol	$C_3H_5F_3O$	2240-88-2	Fluoride	1063
3,3,3-Trifluoropropene	$C_3H_3F_3$	677–21–4	Fluoride	1060
Tri-n-hexylamine	$C_{18}H_{39}N$	102-86-3	Amines	987
1,1,1-Trimethoxyethane	$C_5H_{12}O_3$	1445–45–0	Ethers	930
Trimethoxymethane	$C_4H_{10}O_3$	149–73–5	Ethers	929
Trimethylamine	C ₃ H ₉ N	75–50–3	Amines	986
1,2,3-Trimethylbenzene	C_9H_{12}	526-73-8	Aromat01	864
1,2,4-Trimethylbenzene	C ₉ H ₁₂	95-63-6	Aromat01	864
1,3,5-Trimethylbenzene	C_9H_{12}	108-67-8	Aromat01	864
2,3,4-Trimethyl benzoic acid	$C_{10}H_{12}O_2$	1076–47–7	Acids	959
2,3,5-Trimethyl benzoic acid	$C_{10}H_{12}O_2$	2437–66–3	Acids	959
2,3,6-Trimethyl benzoic acid	$C_{10}H_{12}O_2$	2529–39–7	Acids	959
2,4,5-Trimethyl benzoic acid	$C_{10}H_{12}O_2$	528–90–5	Acids	959,960
2,4,6-Trimetnyl benzoic acid	$C_{10}H_{12}O_2$	480-63-7	Acids	960
3,4,5-Trimethyl benzoic acid	$C_{10}H_{12}O_2$	1076-88-6	Acids	960
2,2,3-Trimethylbutane	C_7H_{16}	464-06-2	q-Alkanes	843
Trimethylbutanedioic acid	$C_7H_{12}O_4$	2103-16-4	Acids	955
2,3,3-Trimethyl-1-butene	C_7H_{14}	594-56-9	s-Alkenes	856
Trimethylene glycol	$C_3H_8O_2$	504-63-2	Alcohols	917
Trimethylene oxide	C₃H ₆ O	503300	Ethers	933
Trimethyl isocyanurate	$C_6H_9N_3O_3$	827167	CyclCHN	1014
2,2,3-Trimethylpentane	C ₈ H ₁₈	564-02-3	q-Alkanes	843,844
2,2,4-Trimethylpentane	C_8H_{18}	540-84-1	q-Alkanes	844
2,3,3-Trimethylpentane	C ₈ H ₁₈	560-21-4	q-Alkanes	844
2,3,4-Trimethylpentane	C ₈ H ₁₈	565-75-3	t-Alkanes	842
2,2,4-Trimethyl-3-pentanone	C ₈ H ₁₆ O	5857–36–3	Ketones	941
2,4,4-Trimethyl-1-pentene	C ₈ H ₁₆	107–39–1	s-Alkenes	857
2,4,4-Trimethyl-2-pentene	C ₈ H ₁₆	107-40-4	s-Alkenes	857
Trimethylsuccinic acid	C ₇ H ₁₂ O ₄	2103–16–4	Acids	955
Trimethylurea	C ₄ H ₁₀ N ₂ O	632-14-4	Ureas	1011
2,4,6-Trinitroaniline	C ₆ H ₄ N ₄ O ₆	489-98-5	Nitros	1030

TABLE 56. Name and Formula Index - Continued

Name	Formula	CAS Registry No.	Family	Page	
1,3,5-Trinitrobenzene	robenzene C ₆ H ₃ N ₃ O ₆ 99-35-4		Nitros	1026	
Trinitromethane	CHN ₃ O ₆	517-25-9	Nitros	1022	
2,4,6-Trinitrophenol	$C_6H_3N_3O_7$	29663-11-4	Nitros	1028	
2,4,6-Trinitrotoluene	$C_7H_5N_3O_6$	118-96-7	Nitros	1027	
Tri-n-nonylamine	C ₂₇ H ₅₇ N	2044-22-6	Amines	987.988	
Tri-n-octylamine	$C_{24}H_{51}N$	1116-76-3	Amines	987	
3,5,7-Trioxanonane	$C_6H_{14}O_3$	111-96-6	Ethers	930,931	
Triphenylamine	$C_{18}H_{15}N$	603-34-9	Amines	988	
Triphenylazidomethane	$C_{19}H_{15}N_3$	14309-25-2	Azides	1001	
1,3,5-Triphenylbenzene	$C_{24}H_{18}$	612-71-5	Aromat02	879	
Triphenylcarbinol	$C_{19}H_{16}O$	76–84–6	Alcohols	917	
Triphenylene	$C_{18}H_{12}$	217-59-4	Aromat02	885	
1,1,1-Triphenylethane	$C_{20}H_{18}$	5271-39-6	Aromat02	877	
1,1,2-Triphenylethane	$C_{20}H_{18}$	1520-42-9	Aromat02	877	
Triphenylethylene	$C_{20}H_{16}$	58-72-0	Aromat02	877	
Triphenylmethane	$C_{19}H_{16}$	519-73-3	Aromat02	876	
Triphenylmethanol	$C_{19}H_{16}O$	76-84-6	Alcohols	917	
Triphenylmethylazide	$C_{19}H_{15}N_3$	14309-25-2	Azides	1001	
Tri-n-propylamine	$C_9H_{21}N$	102-69-2	Amines	987	
Tritriacontane	$C_{33}H_{68}$	630-05-7	n-Alkanes	835	
L-Tyrosine	C ₉ H ₁₁ NO ₃	60–18–4	Amino acids	1018	
U					
Undecane	C ₁₁ H ₂₄	1120-21-4	n-Alkanes	831	
Undecanedioic acid	$C_{11}H_{20}O_4$	1852-04-6	Acids	953	
Undecanenitrile	$C_{11}H_{21}N$	2244-07-7	Nitriles	993,994	
Undecanoic acid	$C_{11}H_{22}O_2$	112-37-8	Acids	947	
Undecanol	$C_{11}H_{24}O$	112-42-5	Alcohols	911	
Undecanolactone	$C_{11}H_{20}O_2$	710-04-3	Esters	975	
6-Undecanone	$C_{11}H_{22}O$	927-49-1	Ketones	940	
Undecylbenzene	$C_{17}H_{28}$	6742-54-7	Aromat01	867	
Undecylic acid	$C_{11}H_{22}O_2$	112-37-8	Acids	947	
Undecylnitrile	$C_{11}H_{21}N$	2244-07-7	Nitriles	993,994	
Urea	CH₄N ₂ O	57–13–6	Ureas	1011	
v					
Valeric acid	$C_5H_{10}O_2$	109-52-4	Acids	946	
γ-Valerolactone	$C_5H_8O_2$	108-29-2	Esters	975	
δ-Valerolactone	$C_5H_8O_2$	542289	Esters	975	
Valeronitrile	C₅H ₉ N	110-59-8	Nitriles	993	
L-Valine	$C_5H_{11}NO_2$	72-18-4	Amino acids	1016	
Valylphenylalanine	$C_{14}H_{20}N_2O_3$	3918-92-1	Amino acids	1021	
Vinyl acetate	C₄H ₆ O ₂	108-05-4	Esters	971	
Vinylcyclohexane	C ₈ H ₁₄	695-12-5	Cyclic03	904	

W,X,Y,Z

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of the Chemical Thermodynamic Properties for Organic Compound at 298.15 K Database. Part I. Hy-

Appendix 1. Groups Derived from Thermodynamic Data for a Single Compound as Its Source

Groups which have emerged from a thermodynamic value for single compound and which are not cyclic structures are characterized by having residuals equal to zero and are listed below in Table 1–1. Cyclic compound which requires a ring strain correction and result in having zero residuals are excuded from this list but can be found in Table 2. Also excluded from this list are any

molecular corrections, such as the *cis* correction, *ortho*, *meta*, and *para* corrections, and corrections for functional groups on adjacent carbon atoms. Compounds which can be described by a single group and cannot be estimated by group additivity, such as methane, formaldehyde, acetonitrile, nitromethane, methyl chloride, etc., are also found in Table 2.

TABLE 1-1. Groups derived from data on a single compound

Group	Source compound
C-(H)(C) ₂ (C _t)	3-Methyl-1-butyne
$C - (C)_2(C_1)_2$	3,3-Dimethylpenta-1,4-diyne
C_d – $(C)(C_B)$	α-Methylstyrene
$C-(H)_2(C_d)(C_B)$	2-Propenylbenzene
$C-(H)(C)(C_d)(C_B)$	1-Methyl-2-propenyl-benzene
C-(O) ₃ (C)	1,1,1-Trimethoxyethane
CO-(H)(CO)	Glyoxal
CO-(H)(C _d)	trans-2-Butenal
$CO-(H)(C_B)$	Benzaldehyde
$CO-(C_p)(CO)$	Benzil
CO-(C)(CO)	Biacetyl
$C-(C)_2(CN)_2$	2,2-Dimethylpropane-1,3-dinitrile
$C-(C)_3(CN)$	2,2-Dimethylpropanenitrile
$C-(C_B)_3(N_3)$	Triphenylmethyl azide
$C-(H)(C)_2(N_A)$	Diisopropyldiazene
C _B -(CNO)	1,4-Benzodinitrile N-oxide
$C-(H)_2(C_B)(NO_2)$	Nitromethylbenzene
$S-(H)(C_B)$	Benzenethiol
$C-(H)_2(C_B)(S)$	Benzyl mercaptan
$S-(C_B)_2$	Diphenyl sulfide
$S-(C_B)(S)$	Diphenyl disulfide
C-(C) ₃ (SO)	tert-Butyl ethyl sulfoxide
SO_2 - $(C_d)_2$	Divinyl sulfone
SO_2 - $(C_B)_2$	Diphenyl sulfone
SO_2 - $(C_B)(SO_2)$	Diphenyl disulfone
CO-(C)(F)	Acctyl fluoridc
C_{t} –(Cl)	1-Chloropropyne
$C-(H)_2(C_B)(Cl)$	Benzyl chloride
CO-(C)(Cl)	Acetyl chloride
$CO-(C_B)(CI)$	Benzoyl chloride
C _t -(Br)	1-Bromopropyne
$C-(H)_2(C_B)(Br)$	Benzyl bromide
CO-(C)(Br)	Acetyl bromide
C-(C) ₃ (I)	2-Iodo-2-methylpropane
C_{t} – (I)	1-Iodopropyne
$C-(H)_2(C_B)(I)$	Benzyl iodide
CO-(C)(I)	Acetyl Iodide
C-(H)(C)(Cl)(F)	1-Chloro-1-fluoroethane
C-(H)(C)(Br)(Cl)	1,2-Dibromo-1,2-dichloro-ethane
$C-(C)(Br)(F)_2$	1,2-Dibromotetrafluoro-ethane
C_d -(Cl)(F)	Chlorotrifluoroethylene

Appendix 2. Comparison of Literature Data for Enthalples and Entropies of Fusion and Enthalpies of Vaporization with the Estimated Differences for $[\Delta_i H^{\circ}(\text{liq}) - \Delta_i H^{\circ}(\text{g})], [\Delta_i H^{\circ}(\text{solid}) - \Delta_i H^{\circ}(\text{liq})], \text{ and } [S^{\circ}(\text{solid}) - S^{\circ}(\text{liq})], \text{ at 298.15 K}$

We have shown that internal consistency exists when comparisons are made between literature data for enthalpies and entropies of fusion and vaporization and the estimated differences for $[\Delta_i H^{\circ}(\text{liq}) - \Delta_i H^{\circ}(g)], [\Delta_i H^{\circ}(\text{solid}) - \Delta_i H^{\circ}(\text{liq})], \text{ and } [S^{\circ}(\text{solid}) - S^{\circ}(\text{liq})], \text{ at 298.15 K.}$

Tables 2-1, 2-2, and 2-3 compare recommended values for the standard enthalpy of vaporization at 298.15 K from 85MAJ/SVO, and differences between $[\Delta_t H^{\circ}(\text{liq}) - \Delta_t H^{\circ}(g)]$ from 86TRC and 69STU/WES with our estimated difference for $[\Delta_t H^{\circ}(\text{liq}) - \Delta_t H^{\circ}(g)]$ for *n*-alkanes, thiols, and alkyl sulfides. General agreement is observed, usually within less than 1.0 kJ mol⁻¹, and shows that $\Delta_{\text{vap}}H^{\circ} = [\Delta_t H^{\circ}(\text{liq}) - \Delta_t H^{\circ}(g)]$ provides a measure of internal consistency for group additivity as applied to these homologous series.

Tables 2-4 and 2-5 compare literature data for 25 organic compounds with their enthalpies and entropies of fusion, corrected to 298.15 K, with our estimated differences for $[\Delta_t H^{\circ}(\text{solid}) - \Delta_t H^{\circ}(\text{liq})]$ and $[S^{\circ}(\text{solid}) - S^{\circ}(\text{liq})]$.

Equations used to correct $\Delta_{\text{fus}}H^{\circ}$ and $\Delta_{\text{fus}}S^{\circ}$ from the melting temperature (T_{m}) to 298.15 K are:

$$\Delta_{\text{fus}}H^{\circ}$$
 at 298.15 K = $\Delta_{\text{fus}}H^{\circ}$ at $T_{\text{m}} + (\Delta C_{p})(298.15 - T_{\text{m}})$

$$\Delta_{\text{fus}}S^{\circ}$$
 at 298.15 K = $\Delta_{\text{fus}}S^{\circ}$ at $T_{\text{m}} + (\Delta C_{p})\ln(298.15/T_{\text{m}})$,

where ΔC_p is the difference between $C_p(\text{liq})$ and $C_p(\text{solid})$ over the temperature range from T_m to 298.15 K.

Comparison of $\Delta_{\text{fus}}H^{\circ}$ corrected to 298.15 K with our estimated difference of $[\Delta_{\text{f}}H^{\circ}(\text{solid}) - \Delta_{\text{f}}H^{\circ}(\text{liq})]$ from the two columns on the right in Table 2–4 results in an average deviation of $\pm 2.7 \text{ kJ·mol}^{-1}$. A similar comparison of $\Delta_{\text{fus}}S^{\circ}$ corrected to 298.15 K with our estimated dif-

ference of $[S^{\circ}(\text{solid}) - S^{\circ}(\text{liq})]$ from the two columns on the right in Table 2-5 results in an average deviation of $\pm 4.7 \text{ J·mol}^{-1} \cdot \text{K}^{-1}$.

Table 2–6 gives a comparison of literature values for $\Delta_{\rm vap}H^{\circ}$ corrected to 298.15 K with our estimated difference of $[\Delta_i H^{\circ}({\rm liq}) \ \Delta_i H^{\circ}({\rm g})]$; the two columns on the right of Table 2–6 should be compared, which result in an average deviation of $\pm 1.6 \ {\rm kJ \cdot mol^{-1}}$. The equation used to correct data on $\Delta_{\rm vap}H^{\circ}$ at the boiling temperature $(T_{\rm b})$ to 298.15 K is:

$$\Delta_{\text{vap}}H^{\circ}$$
 at 298.15 K = $\Delta_{\text{vap}}H^{\circ}$ at $T_{\text{b}} + (\Delta C_{p})(298.15 - T_{\text{b}})$,

where ΔC_p is the difference between C_p (liq) and C_p (g) over the temperature range from T_b to 298.15 K.

Please note that our estimated $[S^{\circ}(g) - S^{\circ}(liq)]$ at 298.15 is not comparable to the entropy of vaporization corrected to 298.15 K because the former also contains conributions for the entropy of compression, $R \ln P$, and for the difference between the ideal and real gas entropies at 298.15 K.

Although the heat capacity in the gas, liquid, and solid phases appears to have a linear character within a given phase at 298.15 K, the experimental heat capacity difference between the liquid/solid phases does not correlate well with the estimated $[C_p(\text{liq}) - C_p(\text{solid})]$ at 298.15 K for several reasons, such as: (1) the inexactness of extrapolation of ΔC_p at the melting or boiling temperatures to 298.15 K, especially if T_m or T_b is significantly far from 298.15 K, (2) premelting phenomena in the region before reaching T_m , (3) solid/solid phase or lambda transitions near T_m , (4) the non-linearity of heat capacity with temperature in the condensed phase, and (5) minima or maxima in the heat capacity between T_m and T_b for some organic liquids.

Table 2-1. Comparison of literature data for $[\Delta_t H^{\circ}(\text{liq}) - \Delta_t H^{\circ}(g)]$ at 298.15 K and enthalpies of vaporization corrected to 298.15 K with estimated $[\Delta_t H^{\circ}(\text{liq}) - \Delta_t H^{\circ}(g)]$ for n-alkanes

n-Alkane	$\Delta_{\text{vap}}H^{\circ}$ (85MAJ/SVO) kJ·mol ⁻¹	$\Delta_t H^{\circ} (1-g)^a$ (86TRC) kJ·mol ⁻¹	$\Delta_{r}H^{\circ}(1-g)^{a}$ (69STU/WES) kJ·mol ⁻¹	$\Delta_l H^{\circ}(1-g)^a$ (this work) kJ·mol ⁻¹
Butane	19.99	21.74	21.46	20.90
Pentane	26.75	26.73	26.78	26.00
Hexane	31.73	31.74	31.63	31.10
Heptane	36.66	36.57	36.61	36.20
Octane	41.53	41.51	41.51	41.30
Nonane	46.43	46.44	46.44	46.40
Decane	51.39	51.37	51.38	51.50
Undecane	56.43	56.35	56.27	56.60
Dodecane	61.51	61.30	60.67	61.70
Tridecane	66.43	66.36	66.19	66.80
Tetradecane	71.30	71.09	71.13	71.90
Pentadecane	76.11	76.19	76.15	77.00
Hexadecane	81.38	81.38	83.01	82.10
Heptadecane	86.02	86.02	85.94	87.20
Octadecane	<u> </u>	91.07	93.97	92.30

 $^{^{}a}\Delta_{f}H^{\circ}(1-g) = [\Delta_{f}H^{\circ}(1iq) - \Delta_{f}H^{\circ}(g)]$

Table 2-2. Comparison of literature data for $[\Delta_t H^{\circ}(\text{liq}) - \Delta_t H^{\circ}(g)]$ at 298.15 K and enthalpies of vaporization corrected to 298.15 K with estimated $[\Delta_t H^{\circ}(\text{liq}) - \Delta_t H^{\circ}(g)]$ for *n*-alkanethiols

Thiol	Δ _{vap} H° (85MAJ/SVO) kJ·mol ⁻¹	$\begin{array}{c} \Delta_t H^{\circ}(1-g)^a \\ (86TRC) \\ kJ \cdot mol^{-1} \end{array}$	$\Delta_l H^{\circ}(l-g)^a$ (69STU/WES) kJ·mol ⁻¹	$\Delta_t H^{\circ}(1-g)^a$ (this work) kJ·mol ⁻¹
Methanethiol	-	23.80	23.81	23.93
Ethanethiol	27.52	27.30	27.53	27.53
Propanethiol	32.05	32.00	32.00	32.63
Butanethiol	37.70	36.50	36.57	36.73
Pentanethiol	41.26	42.00	41.13	42.83
Hexanethiol	· —	45.80	46.61	47.93
Decanethiol	65.48	65.50	65.10	68.33

 $^{^{}a}\Delta_{f}H^{\circ}(l-g) = [\Delta_{f}H^{\circ}(liq) - \Delta_{f}H^{\circ}(g)]$

TABLE 2-3. Comparison of literature data for $[\Delta_t H^*(\text{liq}) - \Delta_t H^*(g)]$ at 298.15 K and enthalples of vaporization corrected to 298.15 K with estimated $[\Delta_t H^*(\text{liq}) - \Delta_t H^*(g)]$ for alkyl sulfides

Sulfide	$\Delta_{\text{vap}}H^{\circ}$ (85MAJ/SVO) kJ·mol ⁻¹	$\Delta_t H^{\circ}(I-g)$ (86TRC) kJ·mol ⁻¹	$\Delta_t H^{\circ}(1-g)$ (69STU/WES) kJ·mol ⁻¹	$\Delta_t H^{\circ}(l-g)$ (this work) $kJ \cdot mol^{-1}$
Dimethyl	27.99	27.90	27.87	27.87
Methyl ethyl	31.99	31.90	31.97	31.47
Methyl propyl	36.31	36.30	36.28	36.57
Methyl n-butyl	41.50	40.70	40.71	40.67
Methyl tert-butyl	35.90	35.90	35.82	34.89
Methyl pentyl	45.25	45.00	45.19	46.77
Diethyl	35.88	35.90	35.86	35.07
Ethyl propyl	40.01	40.10	40.08	40.17
Ethyl n-butyl	45.25	45.20	45.10	45.27
Ethyl tert-butyl	_	39.90	39.33	38.48

 $^{^{}a}\Delta_{f}H^{\circ}(1-g) = [\Delta_{f}H^{\circ}(1-g) - \Delta_{f}H^{\circ}(g)]$

TABLE 2-4. Comparison of literature data for enthalpies of fusion with estimated $[\Delta_t H^{\circ}(\text{solid}) - \Delta_t H^{\circ}(\text{liq})]$ at 298.15 K

Compound	$\Delta_{ m fus} H^{ m o}$ at $T_{ m m}$	Reference	$(\Delta C_p)(\Delta T)$ correction	Δ _{fus} Η° 298.15 K	$\Delta_t H^{\circ}(s-1)^a$ 298.15 K	
	kJ·mol ⁻¹		kJ•mol ^{−1}	kJ·mol ⁻¹	(this work) kJ·mol ⁻¹	
Hexane	13.08	46DOU/HUF	5.15	18.23	12.98	
Heptane	14.04	61HUF/GRO	6.52	20.56	16.66	
2,2,4-Trimethyl-pentane	9.21	40PIT	3.95	13.16	10.71	
Hexadecane	53.36	54FIN/GRO	0.50	53.86	49.78	
Octadecane	60.48	57MES/GUT	-0.23	60.25	57.14	
Benzene	9.87	48OLI/EAT	0.06	9.93	9.78	
Toluene	6.64	62SCO/GUT	5.50	12.14	12.16	
Naphthalene	18.23	57MCC/FIN	- 0.47	17.76	16.50	
Butanol	9.37	65COU/HAL	4.32	13.69	11.85	
Hexanol	15.38	29KEL2	3.08	18.46	19.21	
Tetradecanol	49.40	91STE/CHI	-0.77	48.63	48.65	
1.6-Hexanediol	22.60	91STE/CHI	-1.00	21.60	25.44	
Phenol	11.51	63AND/COU	-1.03	10.48	9.04	
Diphenyl ether	17.22	51FUR/GIN	-0.11	17.11	14.01	
Benzophenone	18.19	83DEK/VAN	- 1.66	16.53	18.00	
Acetic acid	11.72	82MAR/AND	0.30	12.02	-0.13	
Propionic acid	10.66	82MAR/AND	1.21	11.87	3.63	
Tetradecanoic acid	45.10	82SCH/MIL2	-0.67	44.43	44.11	
Hexadecanoic acid	53.71	82SCH/MIL2	- 0.86	52.85	51.47	
Benzoic acid	18.00	51FUR/MCC	-5.64	12.36	12.01	
Aniline	10.54	62HAT/HIL	1.70	12.24	10.50	
Benzonitrile	10.98	84LEB/BYK	0.73	11.71	9.33	
Methyl phenyl sulfide	14.84	74MES/FIN	2.18	17.02	16.87	
Chlorobenzene	9.56	375 TU	1.28	10.84	7.95	
Bromobenzene	10.70	75MAS/SCO	1.76	12.46	10.80	

^a $\Delta_t H^{\circ}(s-1) = [\Delta_t H^{\circ}(solid) - \Delta_t H^{\circ}(liq)]$

TABLE 2-5. Comparison of literature data for entropies of fusion with estimated [S°(solid) S°(liq)] at 298.15 K

Compound	$\Delta_{\mathrm{fus}} S^{\circ}$ at T_{m}	Reference	$(\Delta C_p) \ln(T/T_{\rm m})$	Δ _{fus} ς° 298.15 K	S°(s-l) _a 298.15 K	
	J·mol ⁻¹ ·K ⁻¹		J·mol-1·K-1	J·mol ⁻¹ ·K ⁻¹	(this work) J·mol ⁻¹ ·K ⁻¹	
Hexane	73.55	46DOU/HUF	21.97	95.52	90.70	
Heptane	76.90	61HUF/GRO	27.64	104.54	100.07	
2,2,4-Trimethyl-pentane	55.56	40PIT	17.51	73.07	69.96	
Hexadecane	183.15	54FIN/GRO	1.70	184.85	184.40	
Octadecane	204.60	57MES/GUT	- 0.77	203.83	203.14	
Benzene	35.40	48OLI/EAT	0.21	35.61	36.72	
Toluene	37.25	62SCO/GUT	23.62	60.87	63.31	
Naphthalene	51.57	57MCC/FIN	- 1.45	50.12	49.88	
Butanol	50.79	65COU/HAL	18.25	69.04	68.48	
Hexanol	68.11	29KEL2	11.81	79.92	87.22	
Tetradecanol	158.84	91STE/CHI	-2.52	156.32	162.18	
1,6-Hexanediol	71.75	91STE/CHI	-3.26	68.49	71.78	
Phenol	36.66	63AND/COU	-3.36	33.30	33.69	
Diphenyl ether	57.38	51FUR/GIN	-0.32	57.06	57.01	
Benzophenone	56.67	83DEK/VAN	-4.11	52.56		
Acetic acid	40.46	82MAR/AND	1.03	41.49	43.70	
Propionic acid	42.19	82MAR/AND	4.42	46.61	58.84	
Tetradecanoic acid	137.79	82SCH/MIL2	-2.15	135.64	161.91	
Hexadecanoic acid	160.02	82SCH/MIL2	- 2.71	157.31	180.65	
Benzoic acid	45.51	51FUR/MCC	-16.36	29.15	· —	
Aniline	39.46	62HAT/HIL	6.02	45.48	45.45	
Benzonitrile	42.16	84LEB/BYK	2.62	44.78	44.90	
Methyl phenyl sulfide	57.85	74MES/FIN	7.88	65.73	-	
Chlorobenzene	41.93	37STU	4.90	46.83	42.70	
Bromobenzene	44.15	75MAS/SCO	6.54	50.69	51.00	

 $^{{}^{}a}S^{o}(s-1) = [S^{o}(solid) - S^{o}(liq)]$

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TABLE 2-6. Comparison of literature data for enthalpies of vaporization with estimated $[\Delta_t H^o(\text{liq}) - \Delta_t H^o(g)]$ at 298.15 K

Compound	$\Delta_{ ext{vap}}H^{\circ}$ at $T_{ ext{b}}$	Reference	$(\Delta C_p)(\Delta T)$	Δ _{vap} H° at 298 K	$\Delta_f H^\circ (1-g)^a$ at 298 K	
	kJ·mol ^{−1}		kJ·mol⁻¹	kJ·mol ⁻¹	(this work) kJ·mol ⁻¹	
Hexane	_	47OSB/GIN	<u> </u>	31.54	31.10	
Heptane	·	47OSB/GIN	<u> </u>	36.54	36.20	
2,2,4-Trimethyl-pentane	31.00	40PIT	4.24	35.24	36.26	
Hexadecane	_	72MOR	· 	81.38	82.10	
Octadecane	_	45PRO/ROS2	_	90.88	92.30	
Benzene	-	47OSB/GIN	<u> </u>	33.84	33.90	
Toluene	. <u>-</u>	45PRO/ROS2	<u> </u>	37.99	38.08	
Naphthalene ^b	_	63MIL	<u> </u>	72.42	70.24	
Butanol	utana)	66WAD2	<u> </u>	52.30	50.62	
Hexanol		66WAD2	_	61.63	60.82	
Tetradecanol ^b		91STE/CHI	<u> </u>	104.90	101.62	
1,6-Hexanediol		91STE/CHI	-	102.90	90.54	
Phenol ^b	45.69	60AND/BID	22.97	68.66	69.60	
Diphenyl ether		72MOR2	_	65.98	65.83	
Benzophenone	_	83DEK/VAN	·	76.68	75.50	
Acetic acid	23.70	85MAJ/SVO	27.90	51.60	48.82	
Propionic acid		85MAJ/SVO	- '	55.00	51.00	
Tetradecanoic acidb	141.00	61DAV/MAL	· -		151.33	
Hexadecanoic acidb	153.55	61DAV/MAL	-	-	168.89	
Benzoic acid ^b	<u> </u>	72MOR2	- .	89.50	91.60	
Aniline	42.44	85MAJ/SVO	13.39	55.83	55.70	
Benzonitrile		59EVA/SKI	·	55.48	56.87	
Methyl phenyl sulfide	. , -	72GOO2		54.31	52.47	
Chlorobenzene	35.19	85MAJ/SVO	5.81	41.00	43.42	
Bromobenzene	_	85MAJ/SVO		41.31	44.70	

 $^{^{}a}\Delta_{t}H^{\circ}(s-1) = [\Delta_{t}H^{\circ}(solid) - \Delta_{t}H^{\circ}(liq)]$ $^{b}Sublimation (c/g)$

Appendix 3. Comparison between Second-Order Group Additivity Approach (Benson) and the Extended Second-Order Group Additivity Approach (Pedley)

A group-additivity scheme has been developed for the estimation of enthalpies of formation in the gas phase at 298.15 K and 101.325 kPa by J. B. Pedley, R. D. Naylor, and S. P. Kirby (86PED/NAY, Chapters 2, 3, and 4) which extends the molecular parameterization of an organic compound in contrast to the limited parameterization used by Benson (76BEN). The more comprehensive account of nearest- and next-to-nearest-neighbor interactions by 86PED/NAY is expected to lead to smaller differences between experimental and estimated values. Because of a higher degree of parameterization and specificity, the scheme becomes more complex. An example of the more comprehensive parameterization can be shown in an examination of the -CH₂- increment in hydrocarbons. The second-order approach of developed by Benson (76BEN) uses the notation: $C-(H)_2(C)_2$, which means that a carbon atom with two hydrogen atoms is also bonded to two other carbon atoms. No restriction is placed upon the kind of carbon atoms the -CH₂- is bonded to in the Benson scheme's notation and there is only one assigned value for a given property for the gas phase. For example, a value of -20.63 kJ/mol has been used for $\Delta_t H^\circ$ in the gas phase for C-(H)₂(C)₂ by 76BEN and also in this work.

The group additivity estimation scheme developed by (86PED/NAY) allows one to specify the nearest and next-to-nearest neighbors in an explicit manner and, hence, has the quality of an extended second-order or third-order approach. The codes used by (86PED/NAY) are different than those used by Benson and are shown in Table 3–1. In Table 3–2, one observes that groups other than -CH₂- also have a significant number of extended parameters for their molecular description. Using the -CH₂- increment as an example, one finds that 86PED/ NAY uses the notation: 2(1 1) for -CH₂- and has assigned 20 possible choices to it for hydrocarbons for estimating the enthalpy of formation in the gas phase. The 20 choices specify discrete carbon groups attached to the -CH₂- group and are shown in Table 3-3. Each of the discrete values for the -CH₂- has the intrinsic quality of accommodating the interactions between two- and threecentre groups, thus, accounting for their differences.

Table 3-4 compares estimated values for the enthalpy of formation of 20 hydrocarbons consisting of some alkanes. alkenes, and alkynes in the gas phase, using the Pedley estimation scheme and using the one in this work developed by Benson and co-workers, with experimentally determined values. Also, provided are selected enthalpies of formation from the tables of thermodynamic properties of hydrocarbons and related compounds compiled in the Thermodynamics Research Center (TRC) at Texas A&M University (86TRC) for comparison with the experimental values used in this work. The difference between the $\Delta_t H^{\circ}$ expt'l and $\Delta_t H^\circ$ est'd from (86PED/NAY) and this work shows average deviations of 0.6 and 0.5 kJ/mol, respectively. We feel that a different set of 20 or more hydrocarbons would give about the same kind of average deviations. We conclude from Table 3-4 that the Pedley approach with extended parameterization of groups and group values shows about the same overall differences in the estimated enthalpies of formation when compared to those calculated in this work.

Table 3–5 is similar to Table 3–4 except that alcohols, ethers, ketones, and acids form the basis of the comparison. In Table 3–5, the difference between the $\Delta_t H^\circ$ expt'l and $\Delta_t H^\circ$ est'd from 86PED/NAY and this work gives average deviations of 1.8 and 1.2 kJ/mol, respectively. Here again, in Table 3–5 the differences reflected in the average deviations suggest that about the same kind of general agreement between experimental and estimated $\Delta_t H^\circ$'s are found as a result of extended parameterization of groups and group values.

The estimation method developed by (86PED/NAY) is clearly described, very systematic, and very scrupulous in its accounting of groups and group interactions. However, from the limited testing and comparisons which we have carried out, we do not see any significant improvement in the differences between experimental and estimated values for the enthalpies of formation in the gas phase. There are differences in the common base of comparison with respect to experimental values as listed in Tables 3–4 and 3–5, however, these tend to be generally small. We have retained any bias in the choice of experimental values used by 86PED/NAY and those used in this work. The selected values for $\Delta_t H^{\circ \circ}$ s from TRC (86TRC, 86TRC2) makes for another interesting comparison with both experimental and estimated values.

Table 3-1. Group and group codes for aliphatic hydrocarbons and aliphatic oxygen compounds (86PED/NAY)

Group name	Group	Pedley code
methyl	- CH ₃	1
methylene	> CH ₂	2
tertiary C	> CH-	3
quaternary C	>C<	4
ethenic C	$=CH_2$	5
subst. ethenic C	= CH-	6
acetylenic C	≡CH	7
subst. acetylenic C	≡ C-	8
allenic	= C =	9
hydroxyl OH	- OH	O 1
ether O	>0	O2
ketone CO	>CO	K2
acid COOH	- COOH	O1(K2)

Table 3-2. Group comparisons for aliphatic hydrocarbons and aliphatic organic oxygen compounds

Group	No. of g			
-	Benson	Pedley	This work	
-CH ₃	1	1	1	
-CH ₂ -	1	24	1	
-CH <	1	19	1	
>C<	1	14	1	
primary -OH	1	4	1	
secondary -OH	1	4	1	
tertiary -OH	1	2	1	
ether O	1	12	1	
ketone CO	1	10	1	
acid -COOH	2	4	2	
Corrections for:				
Alkane gauche	1	0	0	
Alkene gauche	1	0	0	
1,4 repulsion	0	0	1	
1,5 repulsion	1	0	1	
methyl group				
repulsion	0	0	4	
alkene cis	1	0	1	

TABLE 3-3. Group specificity and values for bonding of -CH₂- to two carbon atoms in aliphatic hydrocarbons (86PED/NAY)

		
Pedley notation for -CH ₂ -	specific group equivalent	group value (kJ/mol)
2(1 1) ^a	CH ₃ -CH ₂ -CH ₃	- 20.90
2(2 1)	-CH ₂ -CH ₂ -CH ₃	- 20.80
2(2 2)	-CH ₂ -CH ₂ -CH ₂ -	-20.80
2(3 1)	> CH-CH ₂ -CH ₃	-20.20
2(3 2)b	> CH-CH ₂ -CH ₂ -	-20.10
2(3 3)	> CH-CH ₂ -CH <	- 18.70
2(4 1)	> C-CH₂-CH₃	- 19.60
2(4 2)	\rightarrow C-CH ₂ -CH ₂ -	-16.80
2(4 3)	\Rightarrow C-CH ₂ -CH <	−7.50
2(4 4)	> C-CH2-C ←	4.00
2(6 1)	= CH-CH ₂ -CH ₃	-20.40
2(6 2)	= CH-CH ₂ -CH ₂ -	-21.00
2(6 3)	= CH-CH ₂ -CH <	-22.10
2(6 4)°	= CH-CH ₂ -C ←	- 19.10
2(6 6)	= CH-CH ₂ -CH $=$	- 19.20
2(7 1)	$= C - CH_2 - CH_3$	- 19.60
2(7 2)	$= C-CH_2-CH_2-$	- 23.00
2(7 3)	= C-CH ₂ -CH <	- 18.50
2(7 4)	$= C - CH_2 - C \leftarrow$	- 12.00
2(9 1)	≡ CCH ₂ CH ₃	-20.30

^{*2(1 1)} means a methylene group (2) bonded to two methyl (1) groups. This group identifies propane explicitly.

b2(3 2) means a methylene group (2) bonded to a tertiary carbon atom (3) and another methylene group (2), as in 2-methylpentane.

^{°2(6 4)} means a methylene group (2) bonded to a substituted ethenic group (6) and a quaternary carbon atom (4), as in 4,4-dimethylpentene-1.

TABLE 3-4. Comparison of enthalpies of formation in the gas phase at 298.15 K (in kJ/mol) (alkanes, alkenes, alkynes)

Compound	$\Delta_t H^\circ \text{expt'l}$ (86PED/NAY)	$\Delta_i H^{\circ}$ expt'l (this work)	Δ _t H°selected (86TRC)	$\Delta_t H^\circ$ est'd (86PED/NAY)	$\Delta_t H^\circ$ est'd (this work)
ethane	-83.8	-83.85	-83.82	-83.8	- 84.52
pentane	- 146.9	-146.82	-146.76	- 146.2	- 146.41
2-methylpentane	-174.8	-174.77	-174.55	-174.4	-173.73
3-methylpentane	-172.1	-172.09	-171.97	- 171.6	- 171.47
2,2-dimethyl-pentane	- 205.9	-205.85	-205.81	-204.4	-204.78
octane	- 208.6	- 208.27	- 208.75	-208.6	-208.30
2-methylheptane	-215.4	-215.35	-215.35	-216.0	-214.99
decane	-249.5	-249.66	-249.46	-250.2	-249.56
dodecane	-289.7	- 290.87	-290.72	-291.8	- 290.82
hexadecane	-374.8	-374.76	-374.17	-375.0	-374.34
1-butene	0.1	-0.54	-0.54	0.1	-0.50
1-hexene	-43.5	-41.51	-41.5	- 42.1	- 41.76
trans-3-hexene	-54.4	-53.89	-52.3	- 53.8	- 53.39
trans-4,4-dimethyl-2-pentene	-88.8	-88.78	-90.2	-87.9	- 87.95
1-octene	-81.4	-82.93	-83.6	-83.7	- 83.02
2-methyl-3-ethyl-1-pentene	- 100.3	-100.29	- 100.7	-100.3	- 101.47
1-decene	- 123.4	- 123.34	- 124.7	- 125.3	-124.28
1-hexadecene	-248.5	-249.16	-248.6	-250.1	-248.06
1-butyne	165.2	165.23	165.23	165.2	166.64
2-butyne	145.7	145.14	145.9	145.6	145.68
average deviation	0.55	0.47	•		

Table 3-5. Comparison of enthalpies of formation in the gas phase at 298.15 K (in kJ/mol) (alcohols, ethers, ketones, acids)

Compound	$\Delta_t H^{\circ} \text{expt'l}$ (86PED/NAY)	$\Delta_t H^\circ \text{expt'l}$ (this work)	$\Delta_t H^{\circ}$ selected (86TRC2)	$\Delta_t H^{\circ}$ est'd (86PED/NAY)	$\Delta_t H^{\circ}$ est'd (this work)
1-butanol	- 275.0	- 275.01	- 274.60	- 275.0	- 275.75
2-butanol	- 292.9	-292.90	-292.88	- 292.9	-292.84
1-pentanol	- 294.7	-294.70	-295.58	-295.8	-296.38
1-hexanol	-315.8	-315.90	-316.80	-316.6	-317.01
1-octanol	-355.5	-355.60	-357.00	- 358.2	- 358.27
1-decanol	-396.4	-396.60	-397.40	- 399.8	- 399.53
diethyl ether	-252.1	-252.10	-252.0	-252.1	- 251.74
dipropyl ether	- 292.9	-293.10	-293.1	- 294.9	-293.00
diisopropyl ether	-319.2	-319.40	-319.4	-318.9	-318.42
di-tert-butyl ether	-362.0	-362.00	-362.0	-362.0	- 363.34
2-pentanone	-259.0	-259.05	- 258.9	-259.1	-259.66
2-hexanone	-279.8	-279.79	-279.0	- 279.9	-280.29
2-methyl-3-pentanone	-286.1	-286.10	-286.1	- 286.1	-286.06
5-nonanone	- 344.9	-344.94	-344,9	- 340.1	-343.39
5-undecanone	-387.4	-387.41	-385.1	- 381.7	- 384.65
propanoic acid	- 453.5	-455.70	-452.8	-451.7	-455.64
butanoic acid	- 475.8	-475.80	-473.6	-472.0	-476.27
pentanoic acid	- 491.9	-496.30	−497.	- 492.8	-496.90
octanoic acid	-554.3	-553.90	−553 .	-555.2	-558.79
dodecanoic acid	-642.0	-642.00	−640.	-638.4	-641.31
average deviation	1.84	1.21			