ABRAHAM SOLVATION PARAMETER MODEL: PREDICTION OF ENTHALPIES OF VAPORIZATION AND SUBLIMATION OF MONO-METHYL BRANCHED ALkanes USING MEASUREMENT GAS CHROMATOGRAPHIC DATA

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Abraham model L solute descriptors have been determined for 174 additional mono-methyl branched alkanes based on published linear-programmed gas chromatographic retention indices. Standard molar enthalpies of vaporization and sublimation at 298 K are calculated for the 174 mono-methylated alkanes using the reported solute descriptors and our recently published Abraham model correlations. Calculated vaporization and sublimation enthalpies derived from the Abraham model compare very favorably with values based on a popular atom-group additivity model. Unlike the additivity model the Abraham model gives different predicted values for each mono-methyl alkane having a given C\textsubscript{n}H\textsubscript{2n+2} molecular formula.

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INTRODUCTION

Gas-liquid chromatographic measurements\textsuperscript{1-10} have been used in the indirect determination of both standard molar enthalpies of vaporization, \( \Delta H_{\text{vap,298K}} \), and standard molar enthalpies of sublimation, \( \Delta H_{\text{sub,298K}} \), of organic compounds at 298 K. For example, Hamilton\textsuperscript{1} determined the \( \Delta H_{\text{vap,298K}} \) of eleven herbicide esters based on experimental gas chromatographic retention volumes, \( V_g \) measured on a nonpolar SE-30 stationary phase. The method assumed that the ratio of the enthalpy of vaporization of each herbicide ester to that of the reference compound (which in this case was dibutyl phthalate) was independent of temperature. The \( \Delta H_{\text{vap,298K}} \) of each individual ester herbicide was calculated from the slope of the graph of \( \ln \left( \frac{V_g\text{ester}}{V_g\text{reference}} \right) \) versus the natural logarithm of the vapor pressure of the reference compound at the column temperature \( T \), \( \ln P_{\text{reference},T} \), in accordance to Eqn. (1).

\[
\ln \left( \frac{V_g\text{ester}}{V_g\text{reference}} \right) = 1 - \frac{\Delta H_{\text{vap,298K},\text{ester}}}{\Delta H_{\text{vap,298K},\text{reference}}} \ln P_{\text{reference},T} + C \quad (1)
\]

Peacock and Fuchs\textsuperscript{2-4} developed a method for determining \( \Delta H_{\text{vap,298K}} \) based on solution calorimetric measurements of liquid organic compounds being dissolved in the stationary phase solvent. The enthalpy of vaporization was calculated as the difference in the measured enthalpy of solution of the organic liquid, \( \Delta H_{\text{soln,298K}} \), minus the chromatographically-measured enthalpy of solution of the gaseous compound in the stationary phase liquid. The later value was determined from the variation in the compound’s retention volumes with temperature, and then corrected back to 298 K using liquid-phase and gas-phase heat capacities.

Chickos and coworkers\textsuperscript{5} proposed a method for determination of \( \Delta H_{\text{vap,298K}} \) based on linear plots of the chromatographically-measured \( \Delta H_{\text{soln}} \) values of gaseous reference compounds in the liquid stationary phase versus the compounds’ known \( \Delta H_{\text{vap,298K}} \) values. Enthalpies of vaporization of additional compounds can then be calculated from the linear mathematical relationship established by the reference compounds. The authors demonstrated the applicability of their method using 102 hydrocarbon and mono-functional hydrocarbon derivatives. Enthalpies of vaporization based on the authors’ method differed from published literature values by a standard deviation of 1.27 kJ mol\textsuperscript{-1}. The method was later extended to the determination of \( \Delta H_{\text{sub,298K}} \) by combining \( \Delta H_{\text{vap,298K}} \) values measured by correlation gas chromatography with calorimetric enthalpy of fusion, \( \Delta H_{\text{fus,298K}} \), adjusted to 298 K.\textsuperscript{6} Numerical values of \( \Delta H_{\text{vap,298K}} \) and \( \Delta H_{\text{sub,298K}} \) determined in this fashion depend on the reference compounds used in establishing the \( \Delta H_{\text{soln}} \) versus \( \Delta H_{\text{vap,298K}} \) mathematical correlation.

Our method of obtaining \( \Delta H_{\text{vap,298K}} \) and \( \Delta H_{\text{sub,298K}} \) values is more of a computational method that uses gas chromatographic retention data to calculate Abraham model solute descriptors. Once calculated, the numerical values of the solute descriptors are then used in conjugation with our published Abraham model correlations\textsuperscript{11,12} to calculate the desired \( \Delta H_{\text{vap,298K}} \) and \( \Delta H_{\text{sub,298K}} \) values of organic, organometallic and inorganic compounds. The Abraham solvation parameter model is among the most widely used linear free energy relationship in the prediction of solute properties having chemical and biological significance. To
date predictive mathematical correlations have been reported for describing solute transfer into more than 130 different organic nonelectrolyte mono-solvents\textsuperscript{13-19} and into more than 100 different ionic liquid solvents.\textsuperscript{20-29} Mathematical correlations have also been developed for predicting enthalpies of solvation of organic vapors and inorganic gases into water and 35 common organic solvents\textsuperscript{30-40} blood-to-body tissues/fluids partition coefficients,\textsuperscript{41-45} lethal median concentrations of organic compounds towards fish and other aquatic organisms,\textsuperscript{46-49} nasal pungency,\textsuperscript{50-53} eye irritation thresholds and Draize eye scores,\textsuperscript{53-55} and many other solute properties.\textsuperscript{56-61} More recently the Abraham model has been extended to predicting enthalpies of vaporization\textsuperscript{11} and sublimation\textsuperscript{12} and the vapor pressure of organic and organometallic compounds.\textsuperscript{62}

In the present communication we illustrate the application of the Abraham solvation parameter model in predicting $\Delta H_{\text{vap},298K}$ and $\Delta H_{\text{sub},298K}$ values. First, we calculate the Abraham model solute descriptors of mono-methyl branched alkanes from published gas chromatographic retention indices of Krkosova and co-workers.\textsuperscript{63} Once calculated, the solute descriptors will be substituted into our previously published Abraham model correlations.\textsuperscript{51,12}

\[
\Delta H_{\text{vap},298K} (\text{kj mol}^{-1}) = 6.100 – 7.363 E + 9.733 S \\
+ 4.025 A + 2.123 B + 9.537 L – 1.180 S\cdot S \\
+ 77.871 A \cdot B – 5.781 I_{\text{amine}} – 14.783 I_{\text{non-a,o-diol}} \\
– 17.873 I_{\text{a,o-diol}} \\
(N = 703, SD = 2.09, R^2 = 0.986, F = 4925.6) \\
(2)
\]

\[
\Delta H_{\text{sub},298K} (\text{kj mol}^{-1}) = 13.93 – 16.90 E + 9.66 S + 10.02 A \\
+ 1.82 B + 13.57 L – 0.30 S\cdot S + 35.43 A \cdot B \\
– 0.05 L \cdot L – 9.09 I_{\text{OH,adj}} + 17.26 I_{\text{OH,non}} + 7.37 I_{\text{NH}} \\
(N = 864, SD = 9.94, R^2 = 0.867, F = 503.2) \\
(3)
\]

Thus enabling the estimation of $\Delta H_{\text{vap},298K}$ and $\Delta H_{\text{sub},298K}$ values for those compounds for which solute descriptors are known. Solute descriptors are identified in Eqs. 2 and 3 by the capitalized alphabetical characters, and are defined as follows: the solute excess molar refractivity expressed in units of $(\text{cm}^3\text{ mol}^{-1}) / (\text{mol} E)$; the solute dipolarity/polarizability $(S)$; the overall or summation hydrogen-bond acidity and basicity $(A$ and $B$, respectively); and the logarithm of the gas-to-hexadecane partition coefficient at 298 K $(L)$. Both Abraham model correlations use indicator variables $(I_{\text{amine}}, I_{\text{OH,adj}}, I_{\text{a,o-diol}}, I_{\text{OH,non}}, I_{\text{NH}})$ to improve the predictions or organic compounds having amino- and more than one hydroxy-functional group. Mono-methylalkanes do not contain either of these functional groups, so no further discussion of indicator variables is needed. The two mathematical correlations were developed based on $\Delta H_{\text{vap},298K}$ and $\Delta H_{\text{sub},298K}$ values for $N = 703$ and $N = 864$ compounds, respectively. As indicated by the standard deviation $(SD)$, squared correlations coefficient $(R^2)$, and Fisher F-statistic $(F)$, both Abraham model correlations provide reasonably accurate mathematical correlations of the $\Delta H_{\text{vap},298K}$ and $\Delta H_{\text{sub},298K}$ data for wide range of organic compounds.

Several earlier publications have illustrated the calculation of Abraham model solute descriptors from either liquid-liquid partition coefficients,\textsuperscript{64} or high-performance liquid chromatographic retention data,\textsuperscript{65} or in the case of crystalline nonelectrolyte compounds from saturation solubilities.\textsuperscript{66-70} The latter papers primarily focused on using the calculated solute descriptors to select organic solvents for recrystallization and/or biphasic partitioning systems for liquid extraction. The intended audience of the solubility studies were chemical engineers and industrial working in the chemical manufacturing sector. Recrystallizations and liquid extractions are commonly used purification methods in chemical syntheses. A more recent publication\textsuperscript{71} reported Abraham solute descriptors of terpene esters determined from gas-liquid chromatographic retention data of solutes eluted on several stationary phase liquids. Here the application was to predict the human odor thresholds of the terpene esters. Solute descriptors of terpene hydrocarbons\textsuperscript{72} had been reported previously. There was very little information in the afore-mentioned studies that would attract the attention of chemical thermodynamic experts or computation chemists, which is the intended audience of the current communication. The calculated solute descriptors of mono-methyl branched alkanes will be used to predict thermodynamic properties, namely $\Delta H_{\text{vap},298K}$ and $\Delta H_{\text{sub},298K}$ values. These thermodynamic quantities are required in the calculation of gas-phase standard molar enthalpies of formation from measured enthalpies of combustion, and in describing how the vapour pressure of a compound varies with temperature. Such information is also needed by individuals working in the chemical manufacturing sector.  

**CALCULATION OF ABRAHAM MODEL SOLUTE DESCRIPTORS**

Determination of solute descriptors generally involves constructing a series of Abraham model correlations that involve solute transfer between two condensed phases (Eqn. 4) or solute transfer from the gas phase into a condensed phase (Eqn. 5).

\[
\text{Solute property} = c_p + e_p \cdot E + s_p \cdot S + a_p \cdot A + b_p \cdot B \\
+ \nu_p \cdot V \\
(4)
\]

\[
\text{Solute property} = c_k + e_k \cdot E + s_k \cdot S + a_k \cdot A + b_k \cdot B \\
+ \nu_k \cdot L \\
(5)
\]

Solute properties used in these computations have included the logarithms of partition coefficients, logarithms of molar solubility ratios, logarithms of chromatographic retention factors, and chromatographic retention indices. Two of the solute descriptors, $E$ and $V$ (McGowan volume), can be reasonably estimated from the solute’s molecular structure. For solutes that lack an acidic hydrogen capable of hydrogen-bond formation, the $A$ solute descriptor can be set equal to zero. This leaves either four solute descriptors $(S, A, B$ and $L)$ or three solute descriptors $(S, B$ and $L)$ to be determined from the Abraham model correlations from the measured solute properties.
The numerical values of \( c_p \), \( p_0 \), \( n_p \), \( b_p \), \( \rho_p \), \( \rho_v \), \( \rho_s \), \( \rho_w \), \( b_w \), \( \rho_0 \), and \( k_0 \) in Eqns. 4 and 5 are known as the solute properties are measured in systems having known values of solvent/process coefficients. The set of Abraham model equations are then solved simultaneously to yield numerical descriptor values for the given solute molecule.

In the case of mono-methyl branched alkane solutes the computation is greatly simplified as \( E = 0 \), \( S = 0 \), \( A = 0 \) and \( B = 0 \). Mono-methyl branched alkane solutes possess no excess molar refraction (\( E = 0 \)) or polarity/polarizability (\( S = 0 \)), and are not capable of hydrogen-bond formation (\( A = 0 \) and \( B = 0 \)) with surrounding solvent molecules. Only the \( L \) solute descriptor remains to be calculated. We calculate the \( L \) solute descriptor of the mono-methyl branched alkanes by first establishing a linear relationship between the measured temperature-programmed linear retention indices, \( R_L \), and the \( L \) solute descriptor based on the values for the n-alkanes and 22 of the 196 compounds studied by Krkosova and coworkers\(^6\) for which we have a known \( L \) solute descriptor.

\[
L = 0.505(0.000) (R_L/100) - 0.381(0.007)
\]  

\[(N = 49, SD = 0.022, R^2 = 1.000, F = 1323009)\]

Standard errors in the equation coefficients are given in parenthesis immediately following the respective coefficient. Numerical values for the 49 compounds used in constructing Eqn. (6) are tabulated in Table 1. The derived mathematical relationship then allows us to calculate the \( L \)-solute descriptors of the remaining 174 mono-methyl branched alkanes. These calculations are summarized in the last column of Table 1. Examination of the numerical entries reveals that eqn. (6) provides reasonably accurate back-calculation of the known \( L \) descriptor values as one might expect from the correlation’s small standard deviation, SD = 0.022, and near unity value for the squared correlation coefficient, \( R^2 = 1.000 \).

Table 1. Retention Indices, \( R_L \), and Abraham Model \( L \) Solute Descriptors for n-Alkanes and Mono-methyl Branched Alkanes.

| Compound     | \( R_L \) | \( L \) value | \( L \) value | \( L \) value |
|--------------|-----------|---------------|---------------|--------------|
|              | (database)| (Eqn. 6)      |               |              |
| Butane       | 400.00    | 1.615         | 1.643         |              |
| 2-Methylpropane | 354.77   | 1.409         | 1.414         |              |
| Pentane      | 500.00    | 2.162         | 2.149         |              |
| 2-Methylbutane | 466.23   | 2.013         | 1.978         |              |
| Hexane       | 600.00    | 2.668         | 2.655         |              |
| 2-Methylpentane | 561.31   | 2.503         | 2.459         |              |
| 3-Methylpentane | 578.05   | 2.581         | 2.544         |              |
| Heptane      | 700.00    | 3.173         | 3.161         |              |
| 2-Methyloctane | 662.48   | 3.001         | 2.971         |              |
| 3-Methyloctane | 672.19   | 3.044         | 3.020         |              |
| Octane       | 800.00    | 3.677         | 3.667         |              |
| 2-Methylheptane | 764.32   | 3.480         | 3.486         |              |
| 4-Methylheptane | 765.88   | 3.483         | 3.494         |              |
| 3-Methylheptane | 772.17   | 3.510         | 3.526         |              |
| Nonane       | 900.00    | 4.182         | 4.173         |              |
| 4-Methyloctane | 864.06   | 3.961         | 3.991         |              |
| 2-Methyloctane | 865.00   | 3.966         | 3.996         |              |
| 3-Methyloctane | 871.89   | 3.998         | 4.031         |              |
| Decane       | 1000.00   | 4.686         | 4.679         |              |

5-Methylnonane 961.09 4.432 4.482
4-Methylnonane 962.83 4.441 4.491
2-Methylnonane 965.39 4.453 4.504
3-Methylnonane 972.06 4.486 4.538
Undecane 1100.00 5.191 5.185
5-Methyldecane 1058.94 4.963 4.977
4-Methyldecane 1062.04 4.963 4.993
2-Methyldecane 1065.62 4.981 5.011
3-Methyldecane 1072.06 5.037 5.044
Dodecane 1200.00 5.696 5.691
6-Methylundecane 1156.16 5.469
5-Methylundecane 1157.36 5.475
4-Methylundecane 1161.21 5.495
2-Methylundecane 1165.48 5.516
3-Methylundecane 1172.15 5.550
Tridecane 1300.00 6.200 6.197
6-Methyltridecane 1254.15 5.965
5-Methyltridecane 1256.18 5.975
4-Methyltridecane 1260.75 5.998
2-Methyltridecane 1265.36 6.022
3-Methyltridecane 1272.12 6.056
Tetradecane 1400.00 6.705 6.703
7-Methyltridecane 1351.94
6-Methyltridecane 1352.60
5-Methyltridecane 1355.43
4-Methyltridecane 1360.35
3-Methyltridecane 1365.35
2-Methyltridecane 1372.33
Pentadecane 1500.00 7.209
6-Methylpentadecane 1451.30
5-Methylpentadecane 1451.63
4-Methylpentadecane 1454.71
3-Methylpentadecane 1460.18
2-Methylpentadecane 1465.37
3-Methylpentadecane 1472.51
Hexadecane 1600.00 7.714
7-Methylhexadecane 1548.19
6-Methylhexadecane 1548.85
5-Methylhexadecane 1550.66
4-Methylhexadecane 1554.24
3-Methylhexadecane 1559.97
2-Methylhexadecane 1565.24
Methylpentadecane 1572.67
Heptadecane 1700.00 8.218
8-Methylheptadecane 1646.96
7-Methylheptadecane 1647.63
6-Methylheptadecane 1650.07
5-Methylheptadecane 1653.97
4-Methylheptadecane 1659.91
3-Methylheptadecane 1665.35
2-Methylheptadecane 1672.99
Methylhexadecane 1800.00 8.722
Octadecane 1745.40
9-Methylheptadecane 1745.55
8-Methylheptadecane 1746.93
7-Methylheptadecane 1749.71
6-Methylheptadecane 1753.65
5-Methylheptadecane 1759.94
4-Methylheptadecane 1849.2
3-Methylheptadecane 1852.4
2-Methylheptadecane 1845.1
1-Methylheptadecane 1845.1
0-Methylheptadecane 1845.1

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### Vaporization enthalpy prediction

#### Section E-Research paper

| Compound                  | Enthalpy (kJ/mol) | Value |
|---------------------------|-------------------|-------|
| Tetracosane               | 2344.25           | 11.481|
| Nonadecane                | 2347.92           | 11.499|
| 9-Methyltricosane         | 2352.88           | 11.525|
| 8-Methyltricosane         | 2360.07           | 11.561|
| 7-Methyltricosane         | 2365.04           | 11.586|
| 6-Methyltricosane         | 2374.70           | 11.635|
| 5-Methyltricosane         | 2500.00           | 12.264|
| 4-Methyltricosane         | 2536.54           | 12.454|
| 3-Methyltricosane         | 2536.98           | 12.456|
| 2-Methyltricosane         | 2573.74           | 12.460|
| 11-Methylheptacosane      | 2539.36           | 12.468|
| 10-Methylpentacosane      | 2541.32           | 12.478|
| 9-Methylpentacosane       | 2543.98           | 12.492|
| 8-Methylpentacosane       | 2547.85           | 12.511|
| 7-Methylpentacosane       | 2553.15           | 12.538|
| 6-Methylpentacosane       | 2560.60           | 12.576|
| 5-Methylpentacosane       | 2565.29           | 12.599|
| 4-Methylpentacosane       | 2575.45           | 12.651|
| 3-Methylpentacosane       | 2600.00           | 12.770|
| 13-Methylhexacosane       | 2565.44           | 12.954|
| 12-Methylhexacosane       | 2635.87           | 12.957|
| 11-Methylhexacosane       | 2636.31           | 12.959|
| 10-Methylhexacosane       | 2637.35           | 12.964|
| 9-Methylhexacosane        | 2639.09           | 12.973|
| 8-Methylhexacosane        | 2641.09           | 12.983|
| 7-Methylhexacosane        | 2643.84           | 12.997|
| 6-Methylhexacosane        | 2647.91           | 13.017|
| 5-Methylhexacosane        | 2653.06           | 13.043|
| 4-Methylhexacosane        | 2660.71           | 13.082|
| 3-Methylhexacosane        | 2665.30           | 13.105|
| 2-Methylhexacosane        | 2675.72           | 13.158|
| 1-Methylhexacosane        | 2800.00           | 13.780|
| 14-Methylheptacosane      | 2734.93           | 13.458|
| 13-Methylheptacosane      | 2735.00           | 13.458|
| 12-Methylheptacosane      | 2735.45           | 13.460|
| 11-Methylheptacosane      | 2736.16           | 13.464|
| 10-Methylheptacosane      | 2737.21           | 13.469|
| 9-Methylheptacosane       | 2739.14           | 13.479|
| 8-Methylheptacosane       | 2741.07           | 13.489|
| 7-Methylheptacosane       | 2743.87           | 13.503|
| 6-Methylheptacosane       | 2747.82           | 13.523|
| 5-Methylheptacosane       | 2753.22           | 13.550|
| 4-Methylheptacosane       | 2760.86           | 13.589|
| 3-Methylheptacosane       | 2765.26           | 13.611|
| 2-Methylheptacosane       | 2776.09           | 13.666|
| 1-Methylheptacosane       | 2900.00           | 14.291|
| Nonacosane                | 9(8), 2020        | 273-284|

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**Vaporization enthalpy prediction**

**Section E - Research paper**

**PREDICTION OF STANDARD MOLAR ENTHALPIES OF VAPORIZATION AND SUBLIMATION**

The chromatographic retention measurements performed by Krokosva and coworkers\(^5\) allowed us to have a complete set of solute descriptors for an additional 180 saturated hydrocarbons. Previously we had only the five solute descriptors \((E, S, A, B,\) and \(V)\) needed for Eqn. (4). Published studies have shown, however, that Eqn. (5) of the Abraham model provides the better set of predicted values for several thermodynamic properties such as enthalpies of vaporization\(^11\) and enthalpies of solvation of organic vapours and inorganic gases dissolved both in water and in organic solvents\(^30-40\). Having a complete set of solute descriptors will provide better applicability for these important thermodynamic quantities.

We illustrate the application of the Abraham model by calculating the enthalpies of vaporization (Eqn. 7) and enthalpies of solvation (Eqn. 8) of the 174 mono-methyl branched alkanes for which we have just determined the \(L\) descriptor. For the convenience of the reader we have simplified the predictive expressions to contain only the non-zero terms.

\[
\Delta H_{vap,298K} \text{ (kJ mol}^{-1}\text{)} = 6.100 + 9.537 L \quad (7)
\]

\[
\Delta H_{sub,298K} \text{ (kJ mol}^{-1}\text{)} = 13.93 + 13.57 L - 0.05 L \cdot L \quad (8)
\]

Enthalpy of sublimation predictions given in Table 2, start with the \(C_{20}\)-compounds as most of the smaller compounds is liquid at 298 K. Predicted values of \(\Delta H_{vap,298K}\) are given in Table 3 for all compounds as vaporization enthalpies of compounds that are crystalline at 298 K can be easily determined using the method of correlation gas chromatography.\(^5\)

**Table 2. Comparison of the Enthalpies of Sublimation, \(\Delta H_{sub,298K}\) (kJ mol\(^{-1}\)), Predicted by the Abraham Model Eqn. (6) and the Group-Additivity Method of Naef and Acree (Eqn. 11).**

| Compound                  | \(\Delta H_{sub,298K}\) | Eqn. 8 | \(\Delta H_{sub,298K}\) | Eqn. 11 |
|---------------------------|-------------------------|--------|-------------------------|--------|
| 10-Methylnonadecane       | 137.68                  |        | 140.76                  |        |
| 9-Methylnonadecane        | 137.71                  |        | 140.76                  |        |
| 8-Methylnonadecane        | 137.76                  |        | 140.76                  |        |
| 7-Methylnonadecane        | 137.89                  |        | 140.76                  |        |
| 6-Methylnonadecane        | 138.09                  |        | 140.76                  |        |
| 5-Methylnonadecane        | 138.38                  |        | 140.76                  |        |
| 4-Methylnonadecane        | 138.79                  |        | 140.76                  |        |
| 3-Methylnonadecane        | 139.13                  |        | 140.76                  |        |
| 2-Methylnonadecane        | 139.68                  |        | 140.76                  |        |
| 1-Methylnonadecane        | 144.00                  |        | 147.11                  |        |
| 9-Methylleicosane         | 144.03                  |        | 147.11                  |        |
| 8-Methylleicosane         | 144.10                  |        | 147.11                  |        |
| 7-Methylleicosane         | 144.24                  |        | 147.11                  |        |
| 6-Methylleicosane         | 144.45                  |        | 147.11                  |        |
| 5-Methylleicosane         | 144.75                  |        | 147.11                  |        |
| 4-Methylleicosane         | 145.18                  |        | 147.11                  |        |
| 3-Methylleicosane         | 146.06                  |        | 147.11                  |        |
| 2-Methylleicosane         | 147.11                  |        | 147.11                  |        |
| 1-Methylleicosane         | 150.27                  |        | 153.46                  |        |
| 10-Methylheneicoisan      | 150.27                  |        | 153.46                  |        |
| 9-Methylheneicoisan       | 150.32                  |        | 153.46                  |        |
| 8-Methylheneicoisan       | 150.41                  |        | 153.46                  |        |
| 7-Methylheneicoisan       | 150.56                  |        | 153.46                  |        |
| 6-Methylheneicoisan       | 150.77                  |        | 153.46                  |        |
| 5-Methylheneicoisan       | 151.08                  |        | 153.46                  |        |
| 4-Methylheneicoisan       | 151.51                  |        | 153.46                  |        |
| 3-Methylheneicoisan       | 151.84                  |        | 153.46                  |        |
| 2-Methylheneicoisan       | 152.42                  |        | 153.46                  |        |
| 1-Methylldocosan          | 156.65                  |        | 159.81                  |        |
| 10-Methylldocosan         | 156.55                  |        | 159.81                  |        |
| 9-Methylldocosan          | 156.61                  |        | 159.81                  |        |
| 8-Methylldocosan          | 156.71                  |        | 159.81                  |        |
| 7-Methylldocosan          | 156.86                  |        | 159.81                  |        |
| 6-Methylldocosan          | 157.08                  |        | 159.81                  |        |
| 5-Methylldocosan          | 157.39                  |        | 159.81                  |        |
| 4-Methylldocosan          | 157.83                  |        | 159.81                  |        |
| 3-Methylldocosan          | 158.15                  |        | 159.81                  |        |
| 2-Methylldocosan          | 158.73                  |        | 159.81                  |        |
| 1-Methyltricosan          | 162.74                  |        | 166.16                  |        |
| 12-Methyltricosan         | 162.75                  |        | 166.16                  |        |
| 11-Methyltricosan         | 162.79                  |        | 166.16                  |        |
| 10-Methyltricosan         | 162.92                  |        | 166.16                  |        |
| 9-Methyltricosan          | 162.87                  |        | 166.16                  |        |
Vaporization enthalpy prediction

| Compound             | ∆H_{vap,298K} | ∆H_{vap,298K} |
|----------------------|----------------|----------------|
|                      | Eqn. 7         | Eqn. 10        |
| 8-Methyltricosane    | 162.97         | 166.16         |
| 7-Methyltricosane    | 163.14         | 166.16         |
| 6-Methyltricosane    | 163.37         | 166.16         |
| 5-Methyltricosane    | 163.68         | 166.16         |
| 4-Methyltricosane    | 164.13         | 166.16         |
| 2-Methyltricosane    | 164.44         | 166.16         |
| 3-Methyltricosane    | 165.05         | 166.16         |
| 12-Methyltetradecane | 168.98         | 172.51         |
| 11-Methyltetradecane | 168.99         | 172.51         |
| 10-Methyltetradecane | 169.03         | 172.51         |
| 9-Methyltetradecane  | 169.13         | 172.51         |
| 8-Methyltetradecane  | 169.24         | 172.51         |
| 7-Methyltetradecane  | 169.40         | 172.51         |
| 6-Methyltetradecane  | 169.64         | 172.51         |
| 5-Methyltetradecane  | 169.95         | 172.51         |
| 4-Methyltetradecane  | 170.40         | 172.51         |
| 2-Methyltetradecane  | 170.71         | 172.51         |
| 3-Methylpentadecane  | 171.32         | 172.51         |
| 13-Methylpentadecane | 175.17         | 178.86         |
| 12-Methylpentadecane | 175.17         | 178.86         |
| 11-Methylpentadecane | 175.20         | 178.86         |
| 10-Methylpentadecane | 175.25         | 178.86         |
| 9-Methylpentadecane  | 175.35         | 178.86         |
| 8-Methylpentadecane  | 175.47         | 178.86         |
| 7-Methylpentadecane  | 175.64         | 178.86         |
| 6-Methylpentadecane  | 175.88         | 178.86         |
| 5-Methylpentadecane  | 176.21         | 178.86         |
| 4-Methylpentadecane  | 176.67         | 178.86         |
| 2-Methylpentadecane  | 176.97         | 178.86         |
| 3-Methylpentadecane  | 177.60         | 178.86         |
| 13-Methylhexacosane  | 181.33         | 185.21         |
| 12-Methylhexacosane  | 181.36         | 185.21         |
| 11-Methylhexacosane  | 181.38         | 185.21         |
| 10-Methylhexacosane  | 181.45         | 185.21         |
| 9-Methylhexacosane   | 181.56         | 185.21         |
| 8-Methylhexacosane   | 181.68         | 185.21         |
| 7-Methylhexacosane   | 181.85         | 185.21         |
| 6-Methylhexacosane   | 182.10         | 185.21         |
| 5-Methylhexacosane   | 182.42         | 185.21         |
| 4-Methylhexacosane   | 182.90         | 185.21         |
| 2-Methylhexacosane   | 183.18         | 185.21         |
| 3-Methylhexacosane   | 183.83         | 185.21         |
| 14-Methylheptacosane | 187.50         | 191.56         |
| 13-Methylheptacosane | 187.50         | 191.56         |
| 12-Methylheptacosane | 187.53         | 191.56         |
| 11-Methylheptacosane | 187.57         | 191.56         |
| 10-Methylheptacosane | 187.64         | 191.56         |
| 9-Methylheptacosane  | 187.76         | 191.56         |
| 8-Methylheptacosane  | 187.88         | 191.56         |
| 7-Methylheptacosane  | 188.05         | 191.56         |
| 6-Methylheptacosane  | 188.29         | 191.56         |
| 5-Methylheptacosane  | 188.63         | 191.56         |
| 4-Methylheptacosane  | 189.10         | 191.56         |

Table 3. Comparison of the Enthalpies of Vaporiization, ∆H_{vap,298K} (kJ mol⁻¹), Predicted by the Abraham Model, Eqn. 7, and the Group-Additivity Method of Naef and Aaree, Eqn. 10

| Compound             | ∆H_{vap,298K} | ∆H_{vap,298K} |
|----------------------|----------------|----------------|
|                      | Eqn. 7         | Eqn. 10        |
| 2-Methylheptacosane  | 189.37         | 191.56         |
| 3-Methylheptacosane  | 190.04         | 191.56         |
| 14-Methyloctacosane  | 193.64         | 197.91         |
| 13-Methyloctacosane  | 193.65         | 197.91         |
| 12-Methyloctacosane  | 193.68         | 197.91         |
| 11-Methyloctacosane  | 193.73         | 197.91         |
| 10-Methyloctacosane  | 193.80         | 197.91         |
| 9-Methyloctacosane   | 193.92         | 197.91         |
| 8-Methyloctacosane   | 194.05         | 197.91         |
| 7-Methyloctacosane   | 194.22         | 197.91         |
| 6-Methyloctacosane   | 194.48         | 197.91         |
| 5-Methyloctacosane   | 194.81         | 197.91         |
| 4-Methyloctacosane   | 195.28         | 197.91         |
| 2-Methyloctacosane   | 195.56         | 197.91         |
| 3-Methyldecane       | 196.22         | 197.91         |
| 15-Methylnonacosane  | 199.74         | 204.26         |
| 14-Methylnonacosane  | 199.75         | 204.26         |
| 13-Methylnonacosane  | 199.77         | 204.26         |
| 12-Methylnonacosane  | 199.81         | 204.26         |
| 11-Methylnonacosane  | 199.85         | 204.26         |
| 10-Methylnonacosane  | 199.94         | 204.26         |
| 9-Methylnonacosane   | 200.06         | 204.26         |
| 8-Methylnonacosane   | 200.19         | 204.26         |
| 7-Methylnonacosane   | 200.37         | 204.26         |
| 6-Methylnonacosane   | 200.63         | 204.26         |
| 5-Methylnonacosane   | 200.95         | 204.26         |
| 4-Methylnonacosane   | 201.45         | 204.26         |
| 2-Methylnonacosane   | 201.70         | 204.26         |
| 3-Methylnonacosane   | 202.36         | 204.26         |

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| Compound                  | Vaporization (J/mol) |
|---------------------------|----------------------|
| 6-Methyltetradecane       | 72.52                |
| 5-Methyltetradecane       | 72.67                |
| 4-Methyltetradecane       | 72.93                |
| 2-Methyltetradecane       | 73.18                |
| 3-Methyltetradecane       | 73.53                |
| 8-Methylpentadecane       | 77.18                |
| 7-Methylpentadecane       | 77.21                |
| 6-Methylpentadecane       | 77.30                |
| 5-Methylpentadecane       | 77.47                |
| 4-Methylpentadecane       | 77.75                |
| 2-Methylpentadecane       | 78.00                |
| 3-Methylpentadecane       | 78.36                |
| 8-Methylhexadecane        | 81.94                |
| 7-Methylhexadecane        | 81.98                |
| 6-Methylhexadecane        | 82.09                |
| 5-Methylhexadecane        | 82.28                |
| 4-Methylhexadecane        | 82.57                |
| 2-Methylhexadecane        | 82.83                |
| 9-Methylheptadecane       | 86.69                |
| 8-Methylheptadecane       | 86.70                |
| 7-Methylheptadecane       | 86.77                |
| 6-Methylheptadecane       | 86.90                |
| 5-Methylheptadecane       | 87.09                |
| 4-Methylheptadecane       | 87.40                |
| 2-Methylheptadecane       | 87.65                |
| 9-Methyloctadecane        | 91.45                |
| 8-Methyloctadecane        | 91.48                |
| 7-Methyloctadecane        | 91.57                |
| 6-Methyloctadecane        | 91.71                |
| 5-Methyloctadecane        | 91.92                |
| 4-Methyloctadecane        | 92.22                |
| 2-Methyloctadecane        | 92.48                |
| 3-Methyloctadecane        | 92.87                |
| 10-Methylnonadecane       | 96.21                |
| 9-Methylnonadecane        | 96.23                |
| 8-Methylnonadecane        | 96.27                |
| 7-Methylnonadecane        | 96.36                |
| 6-Methylnonadecane        | 96.52                |
| 5-Methylnonadecane        | 96.73                |
| 4-Methylnonadecane        | 97.05                |
| 2-Methylnonadecane        | 97.30                |
| 3-Methylnonadecane        | 97.72                |
| 10-Methyleicosane         | 100.99               |
| 9-Methyleicosane          | 101.02               |
| 8-Methyleicosane          | 101.07               |
| 7-Methyleicosane          | 101.17               |
| 6-Methyleicosane          | 101.34               |
| 5-Methyleicosane          | 101.56               |
| 4-Methyleicosane          | 101.88               |
| 2-Methyleicosane          | 102.13               |
| 3-Methyleicosane          | 102.56               |
| 11-Methylheneicosane      | 105.75               |
| 10-Methylheneicosane      | 105.76               |
| 9-Methylheneicosane       | 105.79               |
| 8-Methylheneicosane       | 105.86               |
| 7-Methylheneicosane       | 105.98               |
| 6-Methylheneicosane       | 106.14               |
| 5-Methylheneicosane       | 106.38               |
| 4-Methylheneicosane       | 106.70               |
| 2-Methylheneicosane       | 106.95               |
| 3-Methylheneicosane       | 107.39               |
| 11-Methylcloicosane       | 110.53               |
| 10-Methylcloicosane       | 110.55               |
| 9-Methylcloicosane        | 110.60               |
| 8-Methylcloicosane        | 110.67               |
| 7-Methylcloicosane        | 110.79               |
| 6-Methylcloicosane        | 110.96               |
| 5-Methylcloicosane        | 111.19               |
| 4-Methylcloicosane        | 111.53               |
| 2-Methylcloicosane        | 111.77               |
| 3-Methylcloicosane        | 112.22               |
| 12-Methyltricosane        | 115.29               |
| 11-Methyltricosane        | 115.30               |
| 10-Methyltricosane        | 115.33               |
| 9-Methyltricosane         | 115.39               |
| 8-Methyltricosane         | 115.47               |
| 7-Methyltricosane         | 115.59               |
| 6-Methyltricosane         | 115.77               |
| 5-Methyltricosane         | 116.01               |
| 4-Methyltricosane         | 116.36               |
| 2-Methyltricosane         | 116.60               |
| 3-Methyltricosane         | 117.06               |
| 12-Methyltetraicosane     | 120.09               |
| 11-Methyltetraicosane     | 120.10               |
| 10-Methyltetraicosane     | 120.13               |
| 9-Methyltetraicosane      | 120.20               |
| 8-Methyltetraicosane      | 120.29               |
| 7-Methyltetraicosane      | 120.42               |
| 6-Methyltetraicosane      | 120.60               |
| 5-Methyltetraicosane      | 120.84               |
| 4-Methyltetraicosane      | 121.19               |
| 2-Methyltetraicosane      | 121.42               |
| 3-Methyltetraicosane      | 121.90               |
| 13-Methylpentacosane      | 124.87               |
| 12-Methylpentacosane      | 124.87               |
| 11-Methylpentacosane      | 124.89               |
| 10-Methylpentacosane      | 124.93               |
| 9-Methylpentacosane       | 125.01               |
| 8-Methylpentacosane       | 125.10               |
| 7-Methylpentacosane       | 125.23               |
Vaporization enthalpy prediction

| Methylpentacosane  | 125.42 | 126.47 |
|--------------------|--------|--------|
| 5-Methylpentacosane | 125.67 | 126.47 |
| 4-Methylpentacosane | 126.03 | 126.47 |
| 2-Methylpentacosane | 126.26 | 126.47 |
| 3-Methylpentacosane | 126.75 | 126.47 |
| 13-Methylnonacosane| 129.65 | 131.23 |
| 12-Methyloctacosane| 129.67 | 131.23 |
| 11-Methyloctacosane| 129.69 | 131.23 |
| 10-Methyloctacosane| 129.74 | 131.23 |
| 9-Methyloctacosane | 129.82 | 131.23 |
| 8-Methyloctacosane | 129.92 | 131.23 |
| 7-Methyloctacosane | 130.05 | 131.23 |
| 6-Methyloctacosane | 130.25 | 131.23 |
| 5-Methyloctacosane | 130.50 | 131.23 |
| 4-Methyloctacosane | 130.86 | 131.23 |
| 2-Methyloctacosane | 131.09 | 131.23 |
| 3-Methylheptacosane| 131.59 | 131.23 |
| 14-Methylheptacosane| 134.45 | 135.99 |
| 13-Methylheptacosane| 134.45 | 135.99 |
| 12-Methylheptacosane| 134.47 | 135.99 |
| 11-Methylheptacosane| 134.51 | 135.99 |
| 10-Methylheptacosane| 134.56 | 135.99 |
| 9-Methylheptacosane | 134.65 | 135.99 |
| 8-Methylheptacosane | 134.74 | 135.99 |
| 7-Methylheptacosane | 134.88 | 135.99 |
| 6-Methylheptacosane | 135.07 | 135.99 |
| 5-Methylheptacosane | 135.33 | 135.99 |
| 4-Methylheptacosane | 135.70 | 135.99 |
| 2-Methylheptacosane | 135.91 | 135.99 |
| 3-Methylheptacosane | 136.43 | 135.99 |
| 14-Methylhexacosane | 139.25 | 140.75 |
| 13-Methylhexacosane | 139.25 | 140.75 |
| 12-Methylhexacosane | 139.28 | 140.75 |
| 11-Methylhexacosane | 139.32 | 140.75 |
| 10-Methylhexacosane | 139.38 | 140.75 |
| 9-Methylhexacosane | 139.47 | 140.75 |
| 8-Methylhexacosane | 139.57 | 140.75 |
| 7-Methylhexacosane | 139.71 | 140.75 |
| 6-Methylhexacosane | 139.90 | 140.75 |
| 5-Methylhexacosane | 140.16 | 140.75 |
| 4-Methylhexacosane | 140.54 | 140.75 |
| 2-Methylhexacosane | 140.76 | 140.75 |
| 3-Methylhexacosane | 141.27 | 140.75 |
| 15-Methyleneicosane | 144.04 | 145.51 |
| 14-Methyleneicosane | 144.04 | 145.51 |
| 13-Methyleneicosane | 144.07 | 145.51 |
| 12-Methyleneicosane | 144.09 | 145.51 |
| 11-Methyleneicosane | 144.13 | 145.51 |
| 10-Methyleneicosane | 144.20 | 145.51 |
| 9-Methyleneicosane | 144.29 | 145.51 |

We are unable to find experimental \( \Delta H_{\text{vap}, 298K} \) and \( \Delta H_{\text{sub}, 298K} \) data in the published chemical literature to compare our calculated values against. What we offer in the way of a comparison is to compare our calculated values against the calculated values of a popular group-additivity method\(^73\) that has been shown to predict \( \Delta H_{\text{vap}, 298K} \) and \( \Delta H_{\text{sub}, 298K} \) values for a wide range of organic and organometallic compounds to within standard deviations of \( SD = 4.30 \text{ kJ mol}^{-1} (N = 3460 \text{ compounds}) \) and \( SD = 10.33 \text{ kJ mol}^{-1} (N = 1866 \text{ compounds}) \), respectively. The basic method (Eqn. 9) sums the contributions that each atomic property, \( \text{sub,298K} \), makes to the given thermodynamic or physical property,

\[
\text{Property} = \sum_{i} A_i a_i + \sum_{j} B_j b_j + C \quad (9)
\]

where \( A_i \) is the number of occurrences of the \( i \text{th atom group} \), \( B_i \) is the number of times each special group occurs, \( a_i \) and \( b_j \) are the numerical values of each atom group and special group, and \( C \) is a constant. For both the \( \Delta H_{\text{vap}, 298K} \) and \( \Delta H_{\text{sub}, 298K} \) computations a \( C_9H_{2n+2} \) mono-methyl branched alkane would be fragmented into 3 sp\(^3\) carbons (with an environment of 3 hydrogen atoms and 1 carbon), 1 sp\(^3\) carbon atom (with an environment of 1 hydrogen atom and 3 carbon atoms), \( n \)-4 sp\(^3\) carbon atoms (with an environment of 2 hydrogen atoms and 2 carbon atoms), and one special alkane group that is multiplied by the number of carbon atoms in the molecule. Numerical values of the groups and constant are different for each property. In Eqsns. (10) and (11) below we have filled in the numerical group values and constants for predicting \( \Delta H_{\text{vap}, 298K} \) (kJ mol\(^{-1}\)) and \( \Delta H_{\text{sub}, 298K} \) (kJ mol\(^{-1}\)) of \( C_9H_{2n+2} \) mono-methyl branched alkanes:

\[
\Delta H_{\text{vap}, 298K} = 3 \times 3.07 + (n-4) \times 4.67 + 3.57 + n \times 0.09 + 8.61 \quad (10)
\]

\[
\Delta H_{\text{sub}, 298K} = 3 \times 5.99 + (n-4) \times 6.88 + 2.28 - n \times 0.53 + 21.03 \quad (11)
\]

Examination of the numerical entries in Tables 2 and 3 reveals that the predictions based on the Abraham model are similar to predictions based on the group-additivity model of Naef and Acree.\(^73\) The group-additivity method though is not able to distinguish between the placement of the methyl group within the molecule, and gives the same predicted values for a given molecular formula. In other words, the predicted values of all methylheicicosane molecules are the same. This limitation is a common feature of most group-additivity and group contribution methods. The Abraham model, on the other hand, does provide different predicted values for a given molecular formula, and does not require
fragmentation of the molecule into atom groups or functional groups. Fragmentation of molecules into functional groups can be difficult at times, particularly in the case of more complex molecules having many different functional groups. Moreover, the solute descriptors for a given molecule can be used to predict many other properties of chemical and biological importance, such as vapour pressure, water-to-organic solvent partition coefficients, gas-to-water partition coefficients, solubility ratios and the infinite dilution activity coefficients of the compound in water.\textsuperscript{74,75}

CONCLUSION

Numerical values of the Abraham model $L$ solute descriptor have been reported for the first time for 174 different $C_{12-20}$ mono-methyl branched alkanes. The numerical values were determined by regression analysis of published linear-programmed gas chromatographic retention indices versus known $L$ solute descriptors of linear alkanes and smaller mono-methylated alkane molecules. Calculated $L$ solute descriptors were used to predict the standard molar enthalpies of vaporization and standard molar enthalpies of sublimation of 174 mono-methyl alkanes at 298 K based on recently published Abraham model correlations.\textsuperscript{11,12} The predicted values compare very favorably with calculated values based on an atom-group additivity model.\textsuperscript{73} Unlike the additivity model the Abraham model gives different predicted values of $\Delta H_{\text{vap,298K}}$ and $\Delta H_{\text{sub,298K}}$ for each mono-methyl alkane having a given $C_{2n+2}$ molecular formula.

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