CALCULATION OF ABRAHAM MODEL L-DESCRIPTOR AND STANDARD MOLAR ENTHALPIES OF VAPORIZATION AND SUBLIMATION FOR C9 - C26 MONO-ALKYL ALKANES AND POLYMETHYL ALKANES

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Abraham model **L** solute descriptors have been determined for 127 additional mono-alkyl alkanes and polymethyl alkanes based on published gas chromatographic retention indices for solutes eluted from a fused-silica capillary column coated with a cross-lined methyl silicone stationary phase. Standard molar enthalpies of vaporization and sublimation at 298 K are calculated for the 127 mono-alkyl alkanes and polymethyl 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 favourably with values based on a popular atom-group additivity model.

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INTRODUCTION

Physicochemical and thermodynamic properties are important input parameters in the design of efficient synthetic methods and purification processes for the commercial preparation of new chemical compounds. Standard molar enthalpies and Gibbs energies of formation can be used to select reaction conditions that optimize product yields, and determine the spontaneity of a chemical reaction at a given temperature and reactant concentrations. Enthalpic and kinetic considerations determine if the reaction mixture needs to be heated or cooled in order for the chemical synthesis to proceed at a controlled reaction rate. Solubility, partition coefficient, vapor pressure, activity coefficient and enthalpy of vaporization data suggest possible purification methods (recrystallization, solvent extraction, fractional distillation) for the chemical product once the synthesis is complete. These represent only a few of the physicochemical and thermodynamic properties needed by individuals working in the chemical manufacturing sector.

Experimental data is readily available for only a small fraction of the more than six billion known chemical compounds. Moreover, in designing industrial manufacturing processes one must consider the properties of liquid mixtures, as well as the properties of individual components that comprise the mixture. Mixture properties such as density, viscosity, surface tension, and vapor pressure depend on the actual concentration of the mixture components. Experimental measurements are both time-consuming and expensive, and it is highly unlikely that there will be a significant increase in the number of experimental values in the near future.

In the absence of actual experimental data, and when measurement is not a viable option, the chemical manufacturing sector has turned to predictive methods as a means to generate the needed input values in design calculations. Many of the current predictive approaches can be classified as either: (1) *Ab-initio* calculational methods; (2) Quantitative Structure Property Relationships (QSPR); or (3) Group Contribution methods. *Ab-initio* methods[1-8] have been successfully applied to compute enthalpies and Gibbs energies of formation, molar heat capacities, enthalpies of solvation, dipole moments, and other properties of molecules of reasonable molecular size. A single computation, however, can take several hours to complete. Various calculation schemes have been employed to reduce the computational time through parameter optimization that allows one to obtain the best possible result for a certain, rather finite, set of test molecules. *Ab-initio* methods are not widely used in process design applications where many computations may be required in order to complete the design of an industrial process.

QSPR relationships are based on finding a mathematical relationship:

$$\varphi = f(MD) \qquad (1)$$

where φ - a physicochemical or thermodynamic property and MD - molecular descriptors

between the desired physicochemical or thermodynamic property and molecular descriptors that describe (or based upon) the molecular characteristics of the molecule. Molecular descriptors can be based upon molecular size,

molecular shape, atom connectivity, atomic volumes and surface areas, components of the dipole and quadruple moment vectors, and calculable local quantities characterizing the reactivity and binding properties (such as atomic charges, atom–atom polarizabilities, molecular orbital energies, and frontier orbital densities). Molecular descriptors are discussed in greater detail elsewhere.[9-11] The mathematical relationship between the descriptors and each physicochemical/thermodynamic property of interest is obtained by curve-fitting the measured experimental data in accordance to Eqn. (1). Properties of any additional compounds are calculated by simply inserting the compound's molecular descriptors into the derived QSPR expression. QSPR expressions have been derived for a large range of physicochemical and thermodynamic properties, including vapor pressure,[12] flash point temperatures,[13,14] Gibbs energies of solvation and Ostwald solubility coefficients,[15,16] liquid viscosity,[17] enthalpies of solvation,[18,19] and liquid and gas molar heat capacities.[20,21]

Group contribution methods belong to a class of empirical property prediction methods that base calculations upon the functional groups or "molecular building blocks" contained within the chemical compound. The molecule is broken down into individual building blocks and the physicochemical and/or thermodynamic property is then estimated as:

$$\varphi = C + \sum_{i}^{groups} n_i G_i \qquad (2)$$

where a constant (C) plus the summation of the product of the number times each group appears in the molecule, n_i, multiplied by the respective group value, G_i. Second- and third-order group terms can be added if necessary to capture subtle structural features that might impact the given property. Such methods assume that the property value for a given function group has the same contribution in all compounds containing the functional group. In other words, the contribution of an ester group would be the same in ethyl acetate as in propyl decanoate. The physicochemical or thermodynamic property of a given chemical compound is thus a function of the contribution of all of the functional groups (or molecular building blocks) needed for the unique representation of the compound's molecular structure.

Molecules can be fragmented into basic organic functional groups (*e.g.*, esters, amides, primary amines, ethers, etc.) or into much smaller atom types and bonded atoms. The key is to find a fragmentation method that results in a general predictive expression for a wide range of chemical compounds or mixtures. Published functional group contribution and atom group additivity methods provide reasonably accurate predictions of enthalpies of combustion,[22] enthalpies of formation,[22-24] standard molar enthalpies of vaporization[25.26] and sublimation,[25,27] solid-liquid total phase entropies,[28,29] surface tensions,[25] isobaric molar heat capacities of liquid and solid organic and organometallic compounds.[30-33] Mathematical expressions for mixtures are more complex and include the mixture compositions as well as terms describing interactions between functional groups on neighboring molecules.[34-38]

The method that we have been promoting in recent years for predicting thermodynamic properties is based on the Abraham solvation parameter model[39-43] which was originally developed to describe solute transfer between two phases.

$$\log(P \text{ or } C_{S,organic}/C_{S,water}) = c_p + e_p \cdot \mathbf{E} + s_p \cdot \mathbf{S} + a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B} + v_p \cdot \mathbf{V} \qquad (3)$$

$$\log(K \text{ or } C_{S,organic}/C_{S,gas}) = c_k + e_k \cdot \mathbf{E} + s_k \cdot \mathbf{S} + a_k \cdot \mathbf{A} + b_k \cdot \mathbf{B} + l_k \cdot \mathbf{L} \qquad (4)$$

Equation (3) describes solute transfer from one condensed phase to another, while Eqn. (4) describes solute transfer from the gas phase into a condensed phase. Solute transfer is described in terms of the logarithms of water-to-organic solvent and gas-to-organic solvent partition coefficients, log P and log K, or in terms of the logarithms of two molar solubility ratios, $C_{S,organic}/C_{S,water}$ and $C_{S,organic}/C_{S,gas}$. The first molar solubility ratio is calculated as the molar solubility of the solute in the organic solvent divided by its aqueous molar solubility, while the second ratio involves a molar gas phase concentration, $C_{s,gas}$. This latter quantity is calculable from the equilibrium vapor pressure of the solute at the system temperature, or can be determined by fitting experimental solubility data in accordance with Eqns. 3 and 4.

The right-hand side of both Abraham model expressions represents the different types of solute-solvent molecular interactions that govern solute transfer processes. Each solute-solvent interaction is quantified as the product of a solute property (**E**, **S**, **A**, **B**, **V** and **L**) multiplied by the complementary solvent property (c_p, e_p, s_p, a_p, b_p, v_p, c_k, e_k, s_k, a_k, b_k, and l_k). Solute descriptors are described as follows: **E** denotes the molar refraction of the given solute in excess of that of a linear alkane having a comparable molecular size; **S** is a combination of the electrostatic polarity and polarizability of the solute; **A** and **B** refer to the respective hydrogen-bond donating and accepting capacities of the dissolved solute; **V** corresponds to the McGowan molecular volume of the solute calculated from atomic sizes and chemical bond numbers; and **L** is the logarithm of the solute's gas-to-hexadecane partition coefficient measured at 298.15 K. The complimentary solvent properties are determined by multi-linear regression analysis of measured log (P or $C_{S,organic}/C_{S,water}$) and log ($K$ or $C_{S,organic}/C_{S,gas}$) values for solutes of known descriptor values. Once the solvent coefficients are known they be used to predict the solubility of additional solutes in the given solvent or log P values for a given water-to-partitioning system. Solubility and partition coefficient data are used in the chemical manufacturing sector to design the chemical separation processes needed to purify the synthesized chemical product. Thus far we have determined solute descriptors for more than 8,000 different organic and organic compounds[44], and have reported Abraham model correlations for more than 130 different water-to-organic solvent and gas-to-organic solvent transfer processes.[39-43] The Gibbs energy of solvation, ΔG_{solv}, is related to the gas-to-liquid partition coefficient through Eqn. (5):

$$\Delta G_{solv} = - RT \ln K \qquad (5)$$

where R denotes the universal gas constant and T is the system temperature. Abraham model correlations are available for predicting the enthalpies of solvation of solutes in several common organic solvents as well.[45-55] Each of our published Abraham model correlations uses the same set of solute descriptors for a given compound, irrespective of the property being predicted.

Our recent modeling efforts have been devoted to developing Abraham model correlations that enable us to predict more physicochemical and thermodynamic properties of organic and organometallic compounds, such as vapor pressures,[56] and enthalpies of vaporization[57] and sublimation.[58] We have now decided to expand our efforts on determining solute descriptors for more chemical compounds. The current communication is devoted to obtaining a complete set of solute descriptors for both the larger C_9 – C_{26} polyalkyl alkanes and polymethyl alkanes so that we can predict their vapor pressures, enthalpies of vaporization and enthalpies of sublimation.

Determination of the solute descriptors of alkane solutes is relatively simple as $E=0$, $S=0$, $A=0$ and $B=0$. 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. The numerical value of the V-solute descriptor is calculable from the number of chemical bonds and the atomic sizes of the atoms contained in the molecular.[59] Only the L solute descriptor remains to be calculated. A recent paper[60] published in the *European Chemical Bulletin* illustrated the determination of the L-solute descriptor of large mono-methyl branched alkanes from measured gas chromatographic retention indices. The identical computational methodology will be followed in the current study using the gas chromatographic Kovats retention indices reported by Kissin and coworkers[61-63] for large alkane and alkene solutes on a fused-silica capillary column coated with a cross-lined methyl silicone stationary phase.

CALCULATION OF ABRAHAM MODEL SOLUTE DESCRIPTORS

The computational method that we will use to calculate the L-solute descriptor involves establishing an Abraham model relationship:

$$RI = c_{ri} + e_{ri} \cdot E + s_{ri} \cdot S + a_{ri} \cdot A + b_{ri} \cdot B + l_{ri} \cdot L \qquad (6)$$

using the measured Kovats retention indices, RI, for those alkane solutes for which we already have a complete set of solute descriptors. Only two of the stationary phase coefficients, c_{ri} and l_{ri}, will need to be determined as the other four terms will not contribute to the computation. Remember that the E, S, A and B solute descriptors of alkane solutes are equal to zero.

The alkane solute that we have available for our linear regression analysis will include the C_5-C_{30} linear alkanes for which the Kovats retention indices are defined to be 100 times the number of carbon atoms, 3-ethyloctane, 4-

ethyloctane, 2,3-dimethyloctane, 2,6-dimethyloctane, 2,7-dimethyloctane, 3,5-dimethyloctane, 3,6-dimethyloctane, 2,6-dimethylheptane, and the 2-methylalkanes for which we recently determined descriptor values.[60] In total we have both retention indices and solute descriptors for 188 different alkane solutes to use in our regression analyses. Analysis of the numerical values in columns 2 and 3 of Table 1 yielded Eqn. 7.

$$L = 0.507(0.000) \cdot (RI/100) - 0.398(0.007) \qquad (7)$$

$$(N = 118, SD = 0.023, R^2 = 1.000, F = 1712340)$$

Standard errors in both equation coefficients are given in parenthesis immediately following the respective coefficient. The statistical information, namely the standard deviation (SD), squared correlations coefficient (R^2), and Fisher F-statistic (F) is provided below the derived correlation.

The derived mathematical relationship allows us to calculate the L solute descriptor of the remaining 127 polyalkyl alkane and polymethyl alkane molecules. These calculations are summarized in the last column of Table 1. Examination of the last two columns of numerical entries in Table 1 reveals that Eqn. (7) provides a very accurate back-calculation of the solute descriptor values used in the regression analysis. The average absolute difference and average difference betwen the experimental-based L-solute descriptor values and those back-calculated from Eqn. (7) were 0.013 and -0.006, respectively.

Table 1. Retention Indices, RI, and Abraham Model L Solute Descriptors for n-Alkanes, Polyalkyl Alkanes and Polymethyl Alkanes.

Compound	RI	L (database)	L Eqn.(7)
Hexane	600.0	2.668	2.644
Heptane	700.0	3.173	3.151
Octane	800.0	3.677	3.658
Nonane	900.0	4.182	4.165
Decane	1000.0	4.686	4.672
Undecane	1100.0	5.191	5.179
Dodecane	1200.0	5.696	5.686
Tridecane	1300.0	6.200	6.193
Tetradecane	1400.0	6.705	6.700
Pentadecane	1500.0	7.209	7.207
Hexadecane	1600.0	7.714	7.714
Heptadecane	1700.0	8.218	8.221
Octadecane	1800.0	8.722	8.728
Nonadecane	1900.0	9.226	9.235
Eicosane	2000.0	9.731	9.742
Heneicosane	2100.0	10.236	10.249
Docosane	2200.0	10.740	10.756
Tricosane	2300.0	11.252	11.263
Tetracosane	2400.0	11.758	11.770
Pentacosane	2500.0	12.264	12.277
Hexacosane	2600.0	12.770	12.784
Heptacosane	2700.0	13.276	13.291
Octacosane	2800.0	13.780	13.798
Nonacosane	2900.0	14.291	14.305
Triacontane	3000.0	14.794	14.812
2-Methyloctane	865.0	3.966	3.988

Compound			
2-Methylnonane	964.0	4.453	4.489
2-Methyldecane	1065.0	4.981	5.002
2-Methylundecane	1164.5	5.516	5.506
2-Methyldodecane	1265.0	6.022	6.016
2-Methyltridecane	1364.5	6.528	6.520
2-Methyltetradecane	1465.0	7.034	7.030
2-Methylpentadecane	1564.0	7.539	7.531
2-Methylhexadecane	1664.5	8.046	8.041
2-Methylheptadecane	1764.0	8.551	8.545
2-Methyloctadecane	1864.5	9.057	9.055
2-Methylnonadecane	1964.0	9.563	9.559
2-Methyleicosane	2064.5	10.070	10.069
2-Methylheneicosane	2164.0	10.575	10.573
2-Methyldocosane	2263.5	11.080	11.078
2-Methyltricosane	2363.0	11.449	11.582
2-Methyltetracosane	2463.0	11.952	12.089
3-Methyloctane	872.0	3.998	4.023
3-Methylnonane	971.0	4.486	4.525
3-Methyldecane	1071.5	5.037	5.035
3-Methylundecane	1172.0	5.550	5.544
3-Methyldodecane	1272.0	6.056	6.051
3-Methyltridecane	1372.0	6.563	6.558
3-Methyltetradecane	1472.5	7.070	7.068
3-Methylpentadecane	1572.0	7.577	7.572
3-Methylhexadecane	1673.0	8.073	8.084
3-Methylheptadecane	1773.5	8.573	8.594
3-Methyloctadecane	1873.5	9.099	9.101
3-Methylnonadecane	1973.7	9.607	9.609
3-Methyleicosane	2074.0	10.114	10.117
3-Methylheneicosane	2174.0	10.621	10.624
3-Methyldocosane	2274.0	11.127	11.131
3-Methyltricosane	2373.7	11.635	11.637
3-Methyltetracosane	2473.7	12.142	12.144
4-Methylnonane	962.0	4.441	4.479
4-Methyldecane	1061.5	4.963	4.984
4-Methylundecane	1161.0	5.495	5.488
4-Methyldodecane	1261.0	5.998	5.995
4-Methyltridecane	1360.0	6.502	6.497
4-Methyltetradecane	1460.5	7.008	7.007
4-Methylpentadecane	1560.0	7.512	7.511
4-Methylhexadecane	1660.5	8.018	8.021
4-Methylheptadecane	1760.0	8.524	8.525
4-Methyloctadecane	1860.2	9.030	9.033
4-Methylnonadecane	1960.2	9.536	9.540
4-Methyleicosane	2060.5	10.043	10.049
4-Methylheneicosane	2160.0	10.549	10.553
4-Methyldocosane	2259.5	11.055	11.058
4-Methyltricosane	2359.0	11.561	11.562
4-Methyltetracosane	2458.5	12.067	12.067
5-Methylnonane	961.0	4.432	4.474
5-Methyldecane	1058.0	4.963	4.966
5-Methylundecane	1156.0	5.475	5.463
5-Methyldodecane	1255.0	5.975	5.965
5-Methyltridecane	1354.0	6.477	6.467
5-Methyltetradecane	1453.8	6.980	6.973
5-Methylpentadecane	1553.6	7.483	7.479
5-Methylhexadecane	1653.4	7.988	7.985
5-Methylheptadecane	1753.2	8.492	8.491
5-Methyloctadecane	1853.0	8.998	8.997
5-Methylnonadecane	1953.2	9.503	9.505
5-Methyleicosane	2053.0	10.009	10.011
5-Methylheneicosane	2153.0	10.514	10.518
5-Methyldocosane	2252.0	11.019	11.020
5-Methyltricosane	2352.5	11.525	11.529
5-Methyltetracosane	2453.0	12.031	12.039
6-Methyldodecane	1254.0	5.965	5.960
6-Methyltetradecane	1451.0	6.964	6.959
6-Methylhexadecane	1650.0	7.968	7.968
6-Methylheptadecane	1749.0	8.473	8.469
6-Methyloctadecane	1848.0	8.977	8.971
6-Methyleicosane	2048.0	9.986	9.985
6-Methylheneicosane	2147.5	10.490	10.490
6-Methyldocosane	2247.0	10.995	10.994
6-Methyltetracosane	2446.5	12.006	12.006
7-Methyltridecane	1351.0	6.460	6.452
7-Methyltetradecane	1450.0	6.957	6.954
7-Methylpentadecane	1548.0	7.456	7.450
7-Methylhexadecane	1646.0	7.956	7.947
7-Methylheptadecane	1745.0	8.458	8.449
7-Methylnonadecane	1944.0	9.465	9.458
7-Methylheneicosane	2143.0	10.473	10.467
7-Methyltricosane	2342.0	11.481	11.476
3-Ethyloctane	961.0	4.467	4.474
3-Ethyldecane	1157.0		5.468
3-Ethyldodecane	1355.0		6.472
3-Ethyltetradecane	1554.0		7.481
3-Ethylhexadecane	1753.0		8.490
3-Ethyloctadecane	1952.0		9.499
3-Ethyleicosane	2152.0		10.513
3-Ethyldocosane	2351.5		11.524
4-Ethyloctane	954.0	4.409	4.439
4-Ethyldecane	1152.0		5.443
4-Ethyldodecane	1348.0		6.436
4-Ethyltetradecane	1548.0		7.450
4-Ethylhexadecane	1747.0		8.459
4-Ethyloctadecane	1947.5		9.476
4-Ethyleicosane	2148.0		10.492
4-Ethyldocosane	2348.0		11.506
5-Ethyldecane	1146.0		5.412
5-Ethyldodecane	1341.0		6.401
5-Ethyltetradecane	1538.0		7.400
5-Ethylhexadecane	1736.0		8.404
5-Ethyloctadecane	1937.0		9.423
5-Ethyleicosane	2137.0		10.437
5-Ethyldocosane	2335.0		11.440
6-Ethyldodecane	1336.0		6.376
6-Ethyltetradecane	1533.0		7.374
6-Ethylhexadecane	1731.0		8.378
6-Ethyloctadecane	1929.0		9.382
6-Ethyleicosane	2129.0		10.396
6-Ethyldocosane	2327.0		11.400
7-Ethyltetradecane	1530.0		7.359
7-Ethylhexadecane	1727.0		8.358
7-Ethyloctadecane	1924.0		9.357
7-Ethyleicosane	2122.0		10.361
7-Ethyldocosane	2320.0		11.364
5-Propyltridecane	1516.0		7.288
5-Propylpentadecane	1712.0		8.282
5-Propylheptadecane	1910.0		9.286
5-Propylnonadecane	2108.0		10.290
7-Propyltridecane	1506.0		7.237
7-Propylpentadecane	1700.0		8.221
7-Propylheptadecane	1898.0		9.225
5-Butyldecane	1313.0		6.259
5-Butyldodecane	1505.0		7.232
5-Butyltetradecane	1699.0		8.216

5-Butylhexadecane	1896.0		9.215
6-Butyldodecane	1498.0		7.197
6-Butyltetradecane	1691.0		8.175
6-Butylhexadecane	1887.0		9.169
7-Butyltetradecane	1688.0		8.160
7-Butylhexadecane	1880.0		9.134
2,3-Dimethyloctane	956.9	4.401	4.453
2,4-Dimethyloctane	919.8		4.265
2,5-Dimethyloctane	926.6		4.300
2,6-Dimethyloctane	936.0	4.304	4.348
2,7-Dimethyloctane	930.6	4.282	4.320
3,5-Dimethyloctane	927.6	4.259	4.305
3,6-Dimethyloctane	942.3	4.331	4.379
4,5-Dimethyloctane	947.8		4.407
2,3-Dimethyldecane	1158.0		5.473
2,4-Dimethyldecane	1115.2		5.256
2,5-Dimethyldecane	1118.5		5.273
2,6-Dimethyldecane	1120.0		5.280
2,7-Dimethyldecane	1125.7		5.309
2,8-Dimethyldecane	1136.8		5.366
2,9-Dimethyldecane	1130.1		5.332
3,5-Dimethyldecane	1118.4		5.272
3,6-Dimethyldecane	1128.8		5.325
3,7-Dimethyldecane	1132.6		5.344
3,8-Dimethyldecane	1143.6		5.400
4,5-Dimethyldecane	1138.0		5.372
4,6-Dimethyldecane	1111.2		5.236
4,7-Dimethyldecane	1120.8		5.284
2,6,10-Trimethylundecane	1276.8		6.075
2,6,10-Trimethyldodecane	1380.6		6.602
2,6,10-Trimethyltridecane	1466.6		7.038
2,6,10-Trimethylpentadecane	1653.6		7.986
2,6,10,14-Tetramethylpentadecane	1711.7		8.280
2,6,10,14-Tetramethylhexadecane	1816.2		8.810
2,6-Dimethylheptane	830.0	3.780	3.810
2,6-Dimethylnonane	1025.3		4.800
3,7-Dimethylnonane	1042.2		4.886
2,6-Dimethylundecane	1216.7		5.771
3,7-Dimethyldodecane	1321.2		6.300
3,7,11-Trimethyltridecane	1485.0		7.131
2,6,10-Trimethyltetradecane	1557.0		7.496
2,6,10,15-Tetramethylhexadecane	1806.0		8.758
2,6,10,15-Tetramethylheptadecane	1913.8		9.305
2,6,10,15-Tetramethyloctadecane	1989.8		9.690
2,6,10,15-Tetramethylnonadecane	2088.5		10.191
2,6,10,15-Tetramethyleicocane	2165.5		10.581
2,6,10,15-Tetramethylheneicosane	2268.0		11.101
2,6,10,15-Tetramethyldocosane	2354.5		11.539
8-Ethylhexadecane	1726.6		8.356
4-Ethylheptadecane	1846.9		8.966
4-Propylhexadecane	1823.4		8.847
5-Propylhexadecane	1808.9		8.773

6-Propylhexadecane	1804.3		8.750
7-Propylhexadecane	1800.0		8.728
8-Propylhexadecane	1798.6		8.721
5-Butylhexadecane	1897.4		9.222
6-Butylhexadecane	1889.7		9.183
7-Butylhexadecane	1884.6		9.157
9-Butylhexadecane	1883.1		9.149
6-Ethylnonadecane	2028.3		9.885
6-Propyloctadecane	2000.0		9.742
6-Butylheptadecane	1987.7		9.680
6-Pentylhexadecane	1979.6		9.639
7-Pentylhexadecane	1972.8		9.604
8-Pentylhexadecane	1971.3		9.596
7-Propylnonadecane	2094.7		10.222
7-Butyloctadecane	2080.5		10.150
7-Pentylheptadecane	2071.7		10.106
7-Hexylhexadecane	2066.0		10.077
8-Hexylhexadecane	2064.2		10.067
8-Methyldocosane	2241.5	11.019	10.966
8-Ethylheneicosane	2218.4		10.849
8-Propyleicosane	2189.5		10.703
8-Butylnonadecane	2174.8		10.628
8-Pentyloctadecane	2166.0		10.584
8-Hexylheptadecane	2160.1		10.554
8-Heptylhexadecane	2158.5		10.546
9-Methyltricosane	2339.4	11.459	11.463
9-Ethyldocosane	2314.9		11.339
9-Propylheneicosane	2285.4		11.189
9-Butyleicosane	2270.4		11.113
9-Pentylnonadecane	2261.2		11.066
9-Hexyloctadecane	2253.4		11.027
9-Heptylheptadecane	2251.7		11.018
10-Methyltetracosane	2436.6	11.957	11.956

PREDICTION OF MOLAR ENTHALPIES OF VAPORIZATION AND MOLAR ENTHALPIES OF SUBLIMATION

A complete set of solute descriptors enables one to estimate a large number of physicochemical and thermodynamic properties using published Abraham model correlations. To date we have reported mathematical expressions for predicting log K and log P values for solutes dissolved in both traditional molecular organic solvents[39-43] and ionic liquid solvents,[64-73] molar solubility ratios,[39-43] blood-to-body tissue/fluid partition coefficients,[74-78] Draize scores and eye irritation thresholds,[79-81] enthalpies of solvation,[45-55] lethal median concentrations of organic compounds towards fish and other aquatic organisms,[82-85] nasal pungency,[79,86-88] vapor pressures,[56] enthalpies of vaporization[57] and sublimation,[58] isobaric molar heat capacities of crystalline, liquid and gaseous organic and organometallic compounds,[89] and many other solute properties.[90-95]

To illustrate the importance of determining solute descriptors for additional compounds, we want to predict a couple of properties that can be used by the scientific community and manufacturing sector. Of the properties for which we have developed Abraham model correlations enthalpies of vaporization and enthalpies of sublimation seem the most logical choice. Large alkanes are not very

soluble in water so the likelihood for the scientific community needing to know the compounds' water-to-organic solvents partition coefficients and lethal molar concentrations towards aquatic organisms is small. Even if large alkanes were to be accidentally released in the environment their aqueous molar concentration would be too small to do significant harm to fish and other aquatic organisms. Also, large alkanes are not pharmaceutical compounds and there is little demand to estimate their distribution in the body. Knowledge of their enthalpies of vaporization and enthalpies of sublimation might be needed, however, in the design of high temperature industrial processes.

Our published Abraham model correlations:[57,58]

$$\Delta H_{vap,298K} \text{ (kJ mol}^{-1}) = 6.100 - 7.363 \text{ } \mathbf{E} + 9.733 \text{ } \mathbf{S}$$
$$+ 4.025 \mathbf{A} + 2.123 \mathbf{B} + 9.537 \mathbf{L} - 1.180 \text{ } \mathbf{S \cdot S}$$
$$+ 77.871 \text{ } \mathbf{A \cdot B} - 5.781 \text{ } \mathbf{I_{amine}} -$$
$$14.783 \text{ } \mathbf{I_{non\text{-}\alpha,\omega\text{-}diol}} - 17.873 \text{ } \mathbf{I_{\alpha,\omega\text{-}diol}} \qquad (8)$$

$$(N = 703, SD = 2.09, R^2 = 0.986, F = 4925.6)$$

and

$$\Delta H_{sub,298K} \text{ (kJ mol}^{-1}) = 13.93 - 16.90 \text{ } \mathbf{E} + 9.66 \text{ } \mathbf{S} +$$
$$10.02 \text{ } \mathbf{A} + 1.82 \text{ } \mathbf{B} + 13.57 \text{ } \mathbf{L} - 0.30 \text{ } \mathbf{S \cdot S} +$$
$$35.43 \text{ } \mathbf{A \cdot B} - 0.05 \text{ } \mathbf{L \cdot L} - 9.09 \text{ } \mathbf{I_{OH,adj}} +$$
$$17.26 \text{ } \mathbf{I_{OH,non}} + 7.37 \text{ } \mathbf{I_{NH}} \qquad (9)$$

$$(N = 864, SD = 9.94, R^2 = 0.867, F = 503.2)$$

provide reasonably accurate predictions the standard molar enthalpies of vaporization, $\Delta H_{vap,298K}$, and standard molar enthalpies of sublimation, $\Delta H_{sub,298K}$, as evidence by the correlations' respective standard deviations of $SD = 2.09$ kJ mol^{-1} and $SD = 9.94$ kJ mol^{-1}, respectively. The larger standard deviations for $\Delta H_{sub,298K}$ result from the difficulty in measuring the low vapor pressures, and from the fact that the measurements were performed at high temperatures and extrapolated back to 298 K.

For the polyalkyl alkanes and polymethyl alkanes considered in the present study only the terms containing the **L** descriptor contribute to the $\Delta H_{vap,298K}$ and $\Delta H_{sub,298K}$. For the convenience of the reader we have simplified the predictive expressions:

$$\Delta H_{vap,298K} \text{ (kJ mol}^{-1}) = 6.100 + 9.537 \text{ } \mathbf{L} \qquad (10)$$

$$\Delta H_{sub,298K} \text{ (kJ mol}^{-1}) = 13.93 + 13.57 \text{ } \mathbf{L} - 0.05 \text{ } \mathbf{L \cdot L} \qquad (11)$$

to contain only the non-zero terms. Enthalpy of sublimation predictions given in Table 2 start with the C_{20}-compounds as most of the smaller compounds are 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[96-100]. Calculated values are given only for those polyalkyl alkanes and polymethyl alkanes for which we just calculated L-descriptor values. Calculated $\Delta H_{vap,298K}$ and $\Delta H_{sub,298K}$ values

for the 2-methyl branched alkanes were reported elsewhere.[60]

Table 2. Comparison of the Enthalpies of Sublimation, $\Delta H_{sub,298K}$ (kJ mol^{-1}), Predicted by the Abraham Model, Eqn. (11), and the Group-Additivity Method of Naef and Acree, Eqn. (14)

Compound	ΔH_{sub} Eqn. (11)	ΔH_{sub} Eqn. (14)
3-Ethyloctadecane	138.32	140.76
3-Ethyleicosane	151.06	153.46
3-Ethyldocosane	163.67	166.16
4-Ethyloctadecane	138.03	140.76
4-Ethyleicosane	150.81	153.46
4-Ethyldocosane	163.45	166.16
5-Ethyloctadecane	137.36	140.76
5-Ethyleicosane	150.11	153.46
5-Ethyldocosane	162.63	166.16
6-Ethyloctadecane	136.84	140.76
6-Ethyleicosane	149.60	153.46
6-Ethyldocosane	162.13	166.16
7-Ethyltetradecane	111.09	115.36
7-Ethylhexadecane	123.85	128.06
7-Ethyloctadecane	136.52	140.76
7-Ethyleicosane	149.16	153.46
7-Ethyldocosane	161.69	166.16
5-Propylheptadecane	135.63	140.76
5-Propylnonadecane	148.27	153.46
7-Propylheptadecane	134.86	140.76
5-Butylhexadecane	134.73	140.76
6-Butylhexadecane	134.15	140.76
7-Butyltetradecane	121.33	128.06
7-Butylhexadecane	133.70	140.76
2,6,10,14-Tetramethylhexadecane	129.60	124.29
2,6,10,15-Tetramethylhexadecane	128.95	124.29
2,6,10,15-Tetramethylheptadecane	135.87	130.64
2,6,10,15-Tetramethyloctadecane	140.73	136.99
2,6,10,15-Tetramethylnonadecane	147.03	143.34
2,6,10,15-Tetramethyleicocane	151.92	149.69
2,6,10,15-Tetramethylheneicosane	158.41	156.04
2,6,10,15-Tetramethyldocosane	163.86	162.39
5-Butylhexadecane	134.82	140.76
6-Butylhexadecane	134.32	140.76
7-Butylhexadecane	134.00	140.76
9-Butylhexadecane	133.90	140.76
6-Ethylnonadecane	143.19	147.11
6-Propyloctadecane	141.38	147.11
6-Butylheptadecane	140.60	147.11
6-Pentylhexadecane	140.08	147.11
7-Pentylhexadecane	139.65	147.11
8-Pentylhexadecane	139.55	147.11
7-Propylnonadecane	147.42	153.46
7-Butyloctadecane	146.52	153.46
7-Pentylheptadecane	145.96	153.46
7-Hexylhexadecane	145.59	153.46

Calculated vaporization enthalpies of alkane derivatives

Section E-Research paper

8-Hexylhexadecane	145.48	153.46		6-Butyldodecane	74.74	78.87
8-Ethylheneicosane	155.27	159.81		6-Butyltetradecane	84.07	88.39
8-Propyleicosane	153.44	159.81		6-Butylhexadecane	93.55	97.91
8-Butylnonadecane	152.51	159.81		7-Butyltetradecane	83.92	88.39
8-Pentyloctadecane	151.95	159.81		7-Butylhexadecane	93.21	97.91
8-Hexylheptadecane	151.57	159.81		2,4-Dimethyloctane	46.78	47.61
8-Heptylhexadecane	151.47	159.81		2,5-Dimethyloctane	47.11	47.61
9-Ethyldocosane	161.37	166.16		4,5-Dimethyloctane	48.13	47.61
9-Propylheneicosane	159.50	166.16		2,3-Dimethyldecane	58.30	57.13
9-Butyleicosane	158.56	166.16		2,4-Dimethyldecane	56.23	57.13
9-Pentylnonadecane	157.98	166.16		2,5-Dimethyldecane	56.39	57.13
9-Hexyloctadecane	157.48	166.16		2,6-Dimethyldecane	56.46	57.13
9-Heptylheptadecane	157.38	166.16		2,7-Dimethyldecane	56.73	57.13

Table 3. Comparison of the Enthalpies of Vaporization, $\Delta H_{vap,298K}$ (kJ mol^{-1}), Predicted by the Abraham Model, Eqn. (10), and the Group-Additivity Method of Naef and Acree, Eqn. (13)

Compound	ΔH_{vap} Eqn. (10)	ΔH_{vap} Eqn. (13)		Compound	ΔH_{vap} Eqn. (10)	ΔH_{vap} Eqn. (13)
3-Ethyldecane	58.25	59.83		2,8-Dimethyldecane	57.27	57.13
3-Ethyldodecane	67.82	69.35		2,9-Dimethyldecane	56.95	57.13
3-Ethyltetradecane	77.44	78.87		3,5-Dimethyldecane	56.38	57.13
3-Ethylhexadecane	87.07	88.39		3,6-Dimethyldecane	56.88	57.13
3-Ethyloctadecane	96.69	97.91		3,7-Dimethyldecane	57.07	57.13
3-Ethyleicosane	106.36	107.43		3,8-Dimethyldecane	57.60	57.13
3-Ethyldocosane	116.01	116.95		4,5-Dimethyldecane	57.33	57.13
4-Ethyldecane	58.01	59.83		4,6-Dimethyldecane	56.03	57.13
4-Ethyldodecane	67.48	69.35		4,7-Dimethyldecane	56.50	55.53
4-Ethyltetradecane	77.15	78.87		2,6,10-Trimethylundecane	64.04	63.95
4-Ethylhexadecane	86.78	88.39		2,6,10-Trimethyldodecane	69.06	68.71
4-Ethyloctadecane	96.47	97.91		2,6,10-Trimethyltridecane	73.22	73.47
4-Ethyleicosane	106.17	107.43		2,6,10-Trimethylpentadecane	82.26	82.99
4-Ethyldocosane	115.84	116.95		2,6,10,14-Tetramethylpentadecane	85.07	85.05
5-Ethyldecane	57.72	59.83		2,6,10,14-Tetramethylhexadecane	90.12	89.81
5-Ethyldodecane	67.15	69.35		2,6-Dimethylnonane	51.88	52.37
5-Ethyltetradecane	76.67	78.87		3,7-Dimethylnonane	52.70	52.37
5-Ethylhexadecane	86.24	88.39		2,6-Dimethylundecane	61.13	61.89
5-Ethyloctadecane	95.96	97.91		3,7-Dimethyldodecane	66.19	66.65
5-Ethyleicosane	105.63	107.43		3,7,11-Trimethyltridecane	74.11	73.47
5-Ethyldocosane	115.21	116.95		2,6,10-Trimethyltetradecane	77.59	78.23
6-Ethyldodecane	66.90	69.35		2,6,10,15-Tetramethylhexadecane	89.63	89.81
6-Ethyltetradecane	76.43	78.87		2,6,10,15-Tetramethylheptadecane	94.84	94.57
6-Ethylhexadecane	86.00	88.39		2,6,10,15-Tetramethyloctadecane	98.52	99.33
6-Ethyloctadecane	95.58	97.91		2,6,10,15-Tetramethylnonadecane	103.29	104.09
6-Ethyleicosane	105.25	107.43		2,6,10,15-Tetramethyleicocane	107.01	108.85
6-Ethyldocosane	114.82	116.95		2,6,10,15-Tetramethylheneicosane	111.97	113.61
7-Ethyltetradecane	76.28	78.87		2,6,10,15-Tetramethyldocosane	116.15	118.37
7-Ethylhexadecane	85.81	88.39		8-Ethylhexadecane	85.79	88.39
7-Ethyloctadecane	95.33	97.91		4-Ethylheptadecane	91.61	93.15
7-Ethyleicosane	104.91	107.43		4-Propylhexadecane	90.47	93.15
7-Ethyldocosane	114.48	116.95		5-Propylhexadecane	89.77	93.15
5-Propyltridecane	75.61	78.87		6-Propylhexadecane	89.55	93.15
5-Propylpentadecane	85.08	88.39		7-Propylhexadecane	89.34	93.15
5-Propylheptadecane	94.66	97.91		8-Propylhexadecane	89.27	93.15
5-Propylnonadecane	104.23	107.43		5-Butylhexadecane	94.05	97.91
7-Propyltridecane	75.12	78.87		6-Butylhexadecane	93.68	97.91
7-Propylpentadecane	84.50	88.39		7-Butylhexadecane	93.43	97.91
7-Propylheptadecane	94.08	97.91		9-Butylhexadecane	93.36	97.91
5-Butyldecane	65.79	69.35		6-Ethylnonadecane	100.38	102.67
5-Butyldodecane	75.07	78.87		6-Propyloctadecane	99.01	102.67
				6-Butylheptadecane	98.41	102.67
5-Butyltetradecane	84.46	88.39		6-Pentylhexadecane	98.02	102.67
				7-Pentylhexadecane	97.69	102.67
5-Butylhexadecane	93.98	97.91		8-Pentylhexadecane	97.62	102.67
				7-Propylnonadecane	103.59	107.43
				7-Butyloctadecane	102.90	107.43
				7-Pentylheptadecane	102.48	107.43
				7-Hexylhexadecane	102.20	107.43
				8-Hexylhexadecane	102.11	107.43

Eur. Chem. Bull. **2020**, *9(10)*, 317-328   http://dx.doi.org/10.17628/ecb.2020.9.317-328   323

8-Ethylheneicosane	109.57	112.19
8-Propyleicosane	108.17	112.19
8-Butylnonadecane	107.46	112.19
8-Pentyloctadecane	107.04	112.19
8-Hexylheptadecane	106.75	112.19
8-Heptylhexadecane	106.67	112.19
9-Ethyldocosane	114.24	116.95
9-Propylheneicosane	112.81	116.95
9-Butyleicosane	112.08	116.95
9-Pentylnonadecane	111.64	116.95
9-Hexyloctadecane	111.26	116.95
9-Heptylheptadecane	111.18	116.95

We were unable to find experimental $\Delta H_{vap,298K}$ and $\Delta H_{sub,298K}$ 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 proposed by Naef and Acree[25] that has been shown to predict $\Delta H_{vap,298K}$ and $\Delta H_{sub,298K}$ values for a wide range of organic and organometallic compounds to within standard deviations of $SD = 4.30$ kJ mol^{-1} ($N=3,460$ compounds) and $SD = 10.33$ kJ mol^{-1} ($N = 1,866$ compounds), respectively. The basic method sums the contributions that each atomic group makes to the given thermodynamic or physical property:

$$\varphi = \sum_i A_i a_i + \sum_j B_j b_j + C \qquad (12)$$

where A_i is the number of occurrences of the ith atom group, B_j 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.

The atom group-additivity method proposed by Naef and Acree[25] fragments branched alkane molecules into three types of sp^3 hybridized carbon atoms based on the number of each type of atoms bonded to the carbon atom. One of the carbon atom-groups will be bonded to three hydrogen atoms and one carbon atom (CH$_3$ group), a second carbon atom type is bonded to two hydrogen atoms and two carbon atoms (CH$_2$ group), and the third carbon atom type is bonded to one hydrogen atom and three carbon atoms (CH group). There is also one special group that is defined as the number of carbon atoms in the alkane molecule.

In Eqns. (13) and (14) below we have filled in the numerical group values and constants for predicting $\Delta H_{vap,298K}$ and $\Delta H_{sub,298K}$ of C$_n$H$_{2n+2}$ polyalkyl alkanes and polymethyl alkanes:

$\Delta H_{vap,298K}$ (kJ mol^{-1}) = 3.07 n_{CH3} + 4.67 n_{CH2} + 3.57 n_{CH}
    + 0.09 $n_{carbons}$ + 8.61   (13)

and

$\Delta H_{sub,298K}$ (kJ mol^{-1}) = 5.99 n_{CH3} + 6.88 n_{CH2} + 2.28 n_{CH}
    − 0.53 $n_{carbons}$ + 21.03   (14)

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 alkyl-substituted group attached to large carbon atom chain, and gives the same predicted values for a given molecular formula. In other words, the predicted values of all mono-propylhexadecane 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, would provide different predicted values for the different propylhexadecane isomers, 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.

As stated in the Introduction we have elected to promote the Abraham solvation parameter model for the correlation and estimation of physicochemical and thermodynamic properties over the many other QSAR and group contribution methods that have been proposed over the years. Abraham model correlations have been developed for a large number of solute transfer process having chemical, biological, pharmaceutical, and environmental significance. The published QSAR and group contribution methods are applicable to a much smaller number of chemical and biological processes. Moreover, the Abraham model solute descriptors for a given molecule can be used to predict many other properties such as vapor pressure, water-to-organic solvent partition coefficients, gas-to-water partition coefficients, solubility ratios, enthalpies of solvation, molar heat capacities of hydration[101], and the infinite dilution activity coefficients of the compound in water[102,103]. There is no need to calculate a different set of descriptor values for each property that one wishes to predict.

SUMMARY

Abraham model **L**-descriptors have been determined for 127 additional mono-alkyl alkanes and polymethyl alkanes from the published gas chromatographic retention indices for solutes eluted from a fused-silica capillary column coated with a cross-lined methyl silicone stationary phase. The computation is based on establishing a mathematical Abraham model correlation using the measured Kovats retention indices, *RI*, for those alkane solutes for which we already have a complete set of solute descriptors. In total experimental values for 118 different alkanes were used to establish the Abraham model correlation.

Calculated **L**-descriptor values were used to predict the standard molar enthalpies of vaporization and standard molar enthalpies of sublimation of 127 mono-alkyl alkanes and polyalkyl alkanes at 298 K based on recently published Abraham model correlations[57,58]. The predicted values compare very favorably with calculated values based on an atom-group additivity model[25].

Unlike simple atom-additivity and group contribution methods, the Abraham model is able to capture the effect that subtle structural features have on the physicochemical and thermodynamic properties of the molecule.

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