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Enthalpy of solvation correlations for gaseous solutes dissolved in dibutyl ether and ethyl acetate

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Abstract

Data have been assembled from the published literature on the enthalpies of solvation for 68 compounds dissolved in dibutyl ether and for 79 compounds dissolved in ethyl acetate. It is shown that an Abraham solvation equation with five descriptors can be used to correlate the experimental enthalpies of solvation in dibutyl ether and ethyl acetate to within standard deviations of 1.88 and 2.16 kJ/mol, respectively. The derived correlations provide very accurate mathematical descriptions of the measured enthalpy of solvation data at 298 K, which in the case of ethyl acetate span a range of about 71 kJ/mol. Mathematical correlations have also been derived for predicting the enthalpies of solvation in dibutyl ether, ethyl acetate, water and 15 additional organic solvents based on the Goss modified version of the Abraham model. Expressions based on this latter model were found to correlate the experimental enthalpies of solvation to within an overall average standard deviation of 2.29 kJ/mol for the 18 solvents studied.

Keywords: Enthalpy of solvation; Linear free energy relationships; Molecular solute descriptors; Predictive methods

1. Introduction

Quantitative structure-property relationship (QSPR) models represent a consolidated computational method to mathematically correlate physical and thermodynamic properties of chemical compounds to molecular features (called molecular descriptors) that range from structural and topological indices to electronic and quantum-chemical properties. Properties that have been correlated include solute solubilities in both water and in organic solvent media, solute partitioning between water and an immiscible (or partly miscible) organic solvent, enthalpies of solvation, oral bioavailability, human and rat intestinal adsorption of drug molecules, drug distribution from blood to the various body organs, toxicities of organic compounds to several aquatic organisms, and the minimum alveolar concentration for inhalation anesthesia to rats. The molecular descriptors may be of either experimental origin or calculated based solely on molecular structure considerations.

Previously, we have applied the Abraham solvation parameter model to describe the enthalpies of solvation of organic solutes and gases in water, $\Delta H_{\mathrm{Solv,W}}$, [1]

$$\begin{aligned}\Delta H_{\mathrm{Solv,W}}\ (\mathrm{kJ/mol}) = {} & -13.310(0.457) + 9.910(0.814)\mathbf{E} \\ & + 2.836(0.807)\mathbf{S} - 32.010(1.102)\mathbf{A} \\ & - 41.816(0.781)\mathbf{B} - 6.354(0.200)\mathbf{L}\end{aligned} \quad (1)$$

with $N = 368$, S.D. = 3.68, $R^2 = 0.964$, $R^2_{\mathrm{adj}} = 0.964$, $F = 1950.5$.

$$\begin{aligned}\Delta H_{\mathrm{Solv,W}}(\mathrm{kJ/mol}) = {} & -6.952(0.651) + 1.415(0.770)\mathbf{E} \\ & - 2.859(0.855)\mathbf{S} - 34.086(1.225)\mathbf{A} \\ & - 42.686(0.850)\mathbf{B} - 22.720(0.800)\mathbf{V}\end{aligned} \quad (2)$$

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(with $N = 369$, S.D. = 4.04, $R^2 = 0.959$, $R^2_{\text{adj}} = 0.958$, $F = 1688.2$) and in methanol, $\Delta H_{\text{Solv,MeOH}}$, [2]

$$\begin{aligned}\Delta H_{\text{Solv,MeOH}}(\text{kJ/mol}) = &-6.366(0.454) - 2.506(0.898)\mathbf{E}\\ &- 1.807(0.907)\mathbf{S} - 37.692(1.163)\mathbf{A}\\ &- 15.466(0.904)\mathbf{B} - 7.674(0.140)\mathbf{L}\end{aligned} \tag{3}$$

(with $N = 188$, S.D. = 2.749, $R^2 = 0.982$, $R^2_{\text{adj}} = 0.982$, $F = 2039.707$)

$$\begin{aligned}\Delta H_{\text{Solv,MeOH}}(\text{kJ/mol}) = &\ 1.636(0.737) - 11.797(1.103)\mathbf{E}\\ &- 9.336(1.161)\mathbf{S} - 41.378(1.504)\mathbf{A}\\ &- 15.984(1.165)\mathbf{B} - 27.891(0.668)\mathbf{V}\end{aligned} \tag{4}$$

(with $N = 188$, S.D. = 3.549, $R^2 = 0.971$, $R^2_{\text{adj}} = 0.970$, $F = 1211.855$) and in hexane [3], heptane [4], hexadecane [4], cyclohexane [4], benzene [4], toluene [5], carbon tetrachloride [5], chloroform [6], 1,2-dichloroethane [6], ethanol [2], 1-butanol [2], 1-octanol [1], propylene carbonate [7], and dimethyl sulfoxide [7]. Numerical values in parenthesis give the standard error for the respective equation coefficient. Each correlation was based on experimental enthalpy of solvation data for 90 or more different solutes. Here and elsewhere, N corresponds to the number of solutes, R denotes the correlation coefficient, S.D. is the standard deviation and F corresponds to the Fisher F-statistic.

The independent variables in Eqs. (1)–(4) are as follows: **E** is the solute excess molar refraction modeling the solute polarizability due to the n- and/or π-electrons in excess of that of a n-alkane of comparable size, **S** is the solute descriptor for the dipolar/polarizability character of the molecule, **A** and **B** are the solute overall or summation hydrogen bond acidity and basicity, **V** is the McGowan volume, and **L** is the logarithm of the gas phase dimensionless Ostwald coefficient of solute into hexadecane at 298.15 K. The first four descriptors can be regarded as measures of the tendency of the given solute to undergo various solute–solvent interactions. The last descriptor, **L**, is a measure of the solvent cavity term that will accommodate the dissolved solute, and will thus be a measure of solute size. General dispersion interactions are also related to solute size, hence **L** will also describe the general solute–solvent interactions. The model considers solute descriptors to be temperature independent values. In fact the **E** and **L** solute descriptors are defined by experimental properties measured at specified temperatures of 293.15 and 298.15 K, respectively. The regression coefficients and constants were obtained by regression analysis of the experimental data for a given process, which in the case of Eqs. (1)–(4) was the enthalpic change resulting from the transfer of the gaseous solute into the respective liquid solvent

In the present communication, we report the Abraham model correlations for enthalpies of solvation of organic solutes and gases in both ethyl acetate and dibutyl ether. Predictive correlations are also derived for a second QSPR model, namely the Abraham model as modified by Goss [8–12]

$$\Delta H_{\text{Solv}}(\text{kJ/mol}) = \text{c} + \text{s} \cdot \mathbf{S} + \text{a} \cdot \mathbf{A} + \text{b} \cdot \mathbf{B} + \text{l} \cdot \mathbf{L} + \text{v} \cdot \mathbf{V} \tag{5}$$

where the lower case letters c, s, a, b, l and v represent the properties of the solvent. The latter model uses the five Abraham solute descriptors **S**, **A**, **B**, **V** and **L**. The Abraham **E** solute descriptor in equations such as Eqs. (1) and (3) is replaced by the McGowan volume (Abraham **V** solute descriptor), which is easily calculable from the individual atomic sizes and number of bonds in the molecule [13]. In the Abraham model, the **V** descriptor generally appears in the expression for solute transfer between two condensed phases

$$\text{SP} = \text{c} + \text{e} \cdot \mathbf{E} + \text{s} \cdot \mathbf{S} + \text{a} \cdot \mathbf{A} + \text{b} \cdot \mathbf{B} + \text{v} \cdot \mathbf{V} \tag{6}$$

where SP is some property of a series of solutes in a fixed phase. Eq. (6) has been used on few occasions to describe gas-to-condensed phase transfer processes in predictive applications where the **L**-descriptors were not known.

2. Data sets and computational methodology

Our search of the chemical literature found a compilation of the enthalpy of solvation data for 59 solutes dissolved in dibutyl ether [14], plus a large number of papers [15–48] that reported experimental enthalpies of solution of liquid and crystalline organic compounds in the two solvents of interest. The latter data were determined by either direct calorimetric methods or calculated based on the temperature dependence of measured infinite dilution activity coefficient data, and the published values were converted to gas-to-organic solvent enthalpies of transfer by

$$\text{Liquid solutes}: \quad \Delta H_{\text{Solv}} = \Delta H_{\text{Soln}} - \Delta H_{\text{Vap,298K}} \tag{7}$$

$$\text{Crystalline solutes}: \quad \Delta H_{\text{Solv}} = \Delta H_{\text{Soln}} - \Delta H_{\text{Sub,298}} \tag{8}$$

subtracting the solute's standard molar enthalpy of vaporization [49], $\Delta H_{\text{Vap,298K}}$, or standard molar enthalpy of sublimation [50], $\Delta H_{\text{Sub,298K}}$, at 298.15 K.

Based on an initial assessment of the available experimental data, we eliminated from consideration all experimental data that pertained to temperatures outside of the temperature range of 283–318 K. Enthalpies of solvation are temperature dependent, and we did not want to introduce large errors in the database by including experimental data far removed from 298 K. Also excluded were values based on solubility measurements where the equilibrium solid phase might be a solvated form of the solid solute. For several solutes there were multiple, independently determined values. In such cases, we selected direct calorimetric data over indirect values based on the temperature dependence of measured solubilities or infinite dilution activity coefficients. Using the fore-mentioned criteria, 68 molar enthalpies of solvation in dibutyl ether and 79 molar enthalpies of solvation in ethyl acetate were selected for regression analysis. The experimental $\Delta H_{\text{Solv,BE}}$ and $\Delta H_{\text{Solv,EA}}$ values are listed in Tables 1 and 2, respectively.

Table 1
Experimental values of the gas to dibutyl ether solvation enthalpy, $\Delta H_{\text{Solv,BE}}$ (kJ/mol), for 68 solutes, together with the solute descriptors

Solute	**E**	**S**	**A**	**B**	**L**	**V**	Exp	Reference
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	−26.28	[15]
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	−31.12	[15]
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	−36.07	[15]
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	−40.96	[15]
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	−45.73	[15]
Decane	0.000	0.000	0.000	0.000	4.686	1.5176	−50.64	[16]
Dodecane	0.000	0.000	0.000	0.000	5.696	1.7994	−60.12	[15]
Hexadecane	0.000	0.000	0.000	0.000	7.714	2.3630	−79.57	[15]
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.9540	−29.99	[18]
3-Ethylpentane	0.000	0.000	0.000	0.000	3.091	1.0949	−34.90	[14]
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.2358	−34.80	[14]
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	−32.38	[14]
1-Hexene	0.078	0.080	0.000	0.070	2.572	0.9110	−30.70	[19]
1-Octene	0.094	0.080	0.000	0.070	3.568	1.1928	−40.40	[14]
1-Octyne	0.155	0.220	0.090	0.100	3.521	1.1498	−43.22	[14]
2-Octyne	0.225	0.300	0.000	0.100	3.850	1.1498	−44.85	[14]
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	−33.06	[14]
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	−37.85	[14]
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	−42.02	[14]
Mesitylene	0.649	0.520	0.000	0.190	4.344	1.1391	−43.38	[14]
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	−31.24	[14]
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	−35.32	[14]
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	−39.45	[14]
Propan-2-ol	0.212	0.360	0.330	0.560	1.764	0.5900	−39.64	[14]
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	−44.94	[14]
2-Butanol	0.217	0.360	0.330	0.560	2.338	0.7309	−40.65	[14]
2-Methylpropan-1-ol	0.217	0.390	0.370	0.480	2.413	0.7309	−44.58	[14]
tert-Butanol	0.180	0.300	0.310	0.600	1.963	0.7309	−37.13	[14]
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	−48.71	[14]
2,2-Dimethyl-1-propanol	0.220	0.360	0.370	0.530	2.650	0.8718	−40.63	[14]
1-Heptanol	0.211	0.420	0.370	0.480	4.115	1.1536	−59.02	[14]
2-Methyl-2-butanol	0.194	0.300	0.310	0.600	2.630	0.8718	−38.79	[25]
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.7309	−26.69	[25]
Butyl methyl ether	0.045	0.250	0.000	0.440	2.658	0.8718	−32.32	[14]
Methyl *tert*-butyl ether	0.024	0.210	0.000	0.590	2.380	0.8718	−29.00	[25]
Dibutyl ether	0.000	0.250	0.000	0.450	3.924	1.2945	−45.00	[14]
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	−31.03	[14]
Acetone	0.179	0.700	0.040	0.490	1.696	0.5470	−26.02	[14]
Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	−30.74	[14]
Pentan-2-one	0.143	0.680	0.000	0.510	2.755	0.8288	−35.12	[14]
Pentan-3-one	0.154	0.660	0.000	0.510	2.811	0.8288	−35.87	[14]
Hexan-2-one	0.136	0.680	0.000	0.510	3.286	0.9697	−40.01	[14]
Heptan-2-one	0.123	0.680	0.000	0.510	3.760	1.1106	−44.31	[14]
Heptan-4-one	0.110	0.660	0.000	0.510	3.705	1.1106	−44.44	[14]
Octan-2-one	0.108	0.680	0.000	0.510	4.257	1.2515	−49.33	[14]
Nonan-2-one	0.119	0.680	0.000	0.510	4.731	1.3924	−53.95	[14]
Nonan-5-one	0.103	0.660	0.000	0.510	4.698	1.3924	−51.33	[14]
2,2,4,4-Tetramethyl-3-pentanone	0.099	0.560	0.000	0.520	4.370	1.3924	−44.31	[14]
Cyclopentanone	0.373	0.860	0.000	0.520	3.221	0.7202	−38.88	[14]
Cyclohexanone	0.403	0.860	0.000	0.560	3.792	0.8611	−41.58	[14]
Propylamine	0.225	0.350	0.160	0.610	2.141	0.6311	−28.23	[14]
Butylamine	0.224	0.350	0.160	0.610	2.618	0.7720	−32.99	[14]
Diethylamine	0.154	0.300	0.080	0.690	2.395	0.7720	−30.50	[20]
Dibutylamine	0.107	0.300	0.080	0.690	4.349	1.3356	−49.24	[14]
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538	−35.55	[14]
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	−26.78	[14]
1-Chloropentane	0.208	0.380	0.000	0.090	3.223	0.9355	−38.14	[14]
1-Bromobutane	0.360	0.400	0.000	0.120	3.105	0.8472	−36.36	[14]
Nitrobenzene	0.871	1.110	0.000	0.280	4.557	0.8906	−50.95	[14]
Anisole	0.710	0.750	0.000	0.290	3.890	0.9160	−44.53	[14]
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162	−52.90	[14]
Methyl methacrylate	0.245	0.510	0.000	0.440	2.880	0.8445	−36.66	[21]
1,1,2,2-Tetrachloroethane	0.542	0.630	0.100	0.080	3.641	0.8800	−50.12	[22]
3-Methylphenol	0.822	0.880	0.570	0.340	4.310	0.9160	−67.03	[25]
Ttrifluoromethylbenzene	0.225	0.480	0.000	0.100	2.894	0.9104	−37.45	[26]
Hexafluorobenzene	0.088	0.560	0.000	0.010	2.345	0.8226	−33.38	[23]
Benzyl alcohol	0.803	0.870	0.330	0.560	4.221	0.9160	−58.10	[24]
Chloroform	0.425	0.490	0.150	0.020	2.480	0.6167	−37.80	[17]

Table 2
Experimental values of the gas to ethyl acetate solvation enthalpy, $\Delta H_{\text{Solv,EA}}$ (kJ/mol), for 79 solutes, together with the solute descriptors

Solute	**E**	**S**	**A**	**B**	**L**	**V**	Exp	Reference
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	−21.30	[15]
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	−25.69	[15]
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	−29.87	[15]
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	−33.84	[15]
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	−37.61	[15]
Decane	0.000	0.000	0.000	0.000	4.686	1.5176	−41.84	[15]
Undecane	0.000	0.000	0.000	0.000	5.191	1.6585	−48.01	[27]
Dodecane	0.000	0.000	0.000	0.000	5.696	1.7994	−50.04	[15]
Tridecane	0.000	0.000	0.000	0.000	6.200	1.9403	−56.61	[27]
Pentadecane	0.000	0.000	0.000	0.000	7.209	2.2221	−63.65	[27]
Hexadecane	0.000	0.000	0.000	0.000	7.714	2.3630	−66.86	[15]
Heptadecane	0.000	0.000	0.000	0.000	8.218	2.5039	−73.75	[27]
2-Methylpentane	0.000	0.000	0.000	0.000	2.503	0.9540	−23.83	[28]
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.9540	−24.63	[28]
3-Methylhexane	0.000	0.000	0.000	0.000	3.044	1.0949	−29.19	[28]
3-Ethylpentane	0.000	0.000	0.000	0.000	3.091	1.0949	−29.08	[29]
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8024	−27.36	[26]
Acetone	0.179	0.700	0.040	0.490	1.696	0.5470	−30.79	[30]
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	−34.27	[30]
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.8288	−37.78	[32]
2-Hexanone	0.136	0.680	0.000	0.510	3.286	0.9697	−41.55	[32]
2-Heptanone	0.123	0.680	0.000	0.510	3.760	1.1106	−45.94	[30]
4-Heptanone	0.110	0.660	0.000	0.510	3.705	1.1106	−44.39	[30]
2-Octanone	0.108	0.680	0.000	0.510	4.257	1.2515	−49.24	[32]
2-Nonanone	0.119	0.680	0.000	0.510	4.735	1.3924	−54.02	[30]
5-Nonanone	0.103	0.660	0.000	0.510	4.698	1.3924	−51.71	[30]
2,2,4,4-Tetramethyl-3-pentanone	0.099	0.560	0.000	0.520	4.370	1.3924	−43.26	[30]
Cyclohexanone	0.403	0.860	0.000	0.560	3.792	0.8611	−44.02	[30]
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	−31.80	[32]
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	−35.38	[33]
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.5900	−38.81	[34]
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.7309	−43.39	[25]
1-Pentanol	0.219	0.420	0.370	0.480	3.106	0.8718	−47.45	[25]
1-Octanol	0.199	0.420	0.370	0.480	4.619	1.2945	−59.67	[31]
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.5900	−37.14	[34]
2-Methyl-2-butanol	0.194	0.300	0.310	0.600	2.630	0.8718	−41.30	[25]
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.7309	−25.98	[25]
Dibutyl ether	0.000	0.250	0.000	0.450	3.924	1.2945	−40.79	[31]
Butyl methyl ether	0.045	0.250	0.000	0.440	2.658	0.8718	−30.79	[26]
Methyl *tert*-butyl ether	0.024	0.110	0.000	0.630	2.380	0.8718	−29.37	[25]
Methyl heptyl ether	0.048	0.250	0.000	0.450	4.088	1.2945	−43.35	[31]
15-Crown-5	0.410	1.200	0.000	1.750	6.779	1.7025	−79.32	[35]
1-Fluorooctane	-0.020	0.350	0.000	0.100	3.850	1.2538	−46.65	[31]
Chloroform	0.425	0.490	0.150	0.020	2.480	0.6167	−36.90	[17]
2-Chloro-2-methylpropane	0.142	0.300	0.000	0.030	2.273	0.7946	−27.98	[36]
1-Chlorooctane	0.191	0.400	0.000	0.090	4.708	1.3580	−49.00	[31]
2-Bromo-2-methylpropane	0.305	0.290	0.000	0.070	2.609	0.8472	−30.73	[36]
1,2-Dibromoethane	0.747	0.760	0.100	0.170	3.382	0.7404	−41.31	[37]
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	−33.48	[33]
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	−37.49	[26]
Mesitylene	0.649	0.520	0.000	0.190	4.344	1.1391	−45.31	[26]
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854	−55.89	[38]
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3242	−64.40	[39]
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	−76.60	[39]
2,2,2-Trifluoroethanol	0.015	0.600	0.570	0.250	1.224	0.5022	−46.00	[33]
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	−35.14	[50]
3-Methylphenol	0.822	0.880	0.570	0.340	4.310	0.9160	−67.28	[25]
Trifluoromethylbenzene	0.225	0.480	0.000	0.100	2.894	0.9104	−37.70	[26]
Nitrobenzene	0.871	1.110	0.000	0.280	4.557	0.8906	−56.02	[26]
Anisole	0.710	0.750	0.000	0.290	3.890	0.9160	−47.11	[26]
Sulfur dioxide	0.370	0.660	0.280	0.100	0.778	0.3465	−29.71	[40]
Nitric oxide	0.370	0.020	0.000	0.090	−0.590	0.2026	−2.53	[41]
Pyrrole	0.613	0.730	0.410	0.290	2.865	0.5770	−49.53	[42]
N-Methylpyrrole	0.559	0.790	0.000	0.310	2.923	0.7180	−40.46	[42]

Table 2 (*Continued*)

Solute	**E**	**S**	**A**	**B**	**L**	**V**	Exp	Reference
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538	−31.80	[43]
1-Bromoadamantane	1.070	0.900	0.000	0.200	6.130	1.3668	−55.80	[44]
1-Adamantanol	0.940	0.900	0.310	0.660	5.634	1.2505	−63.80	[44]
Salicylamide	1.160	1.650	0.630	0.480	5.910	1.0315	−83.53	[45,46]
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751	−64.43	[32]
Benzaldehyde	0.820	1.000	0.000	0.390	4.008	0.8730	−50.63	[32]
Pyridine	0.631	0.840	0.000	0.520	3.022	0.6753	−39.87	[29]
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162	−59.29	[29]
2-Methylpyridine	0.598	0.750	0.000	0.580	3.422	0.8162	−42.50	[47]
Piperidine	0.422	0.460	0.100	0.690	3.304	0.8043	−39.50	[47]
1-Butylamine	0.224	0.350	0.160	0.610	2.618	0.7720	−34.86	[47]
Acetic acid	0.265	0.640	0.630	0.440	1.816	0.4648	−47.46	[47]
Formic acid	0.343	0.750	0.760	0.330	1.545	0.3239	−48.55	[47]
Trichloroethene	0.524	0.370	0.080	0.030	2.997	0.7146	−36.72	[48]
Tetrachloroethene	0.639	0.440	0.000	0.000	3.584	0.8370	−38.05	[48]

Molecular descriptors for all of the compounds considered in the present study are also tabulated in Tables 1 and 2. The tabulated values came from our solute descriptor database, which now contains values for more than 3500 different organic and organometallic compounds. The descriptors were obtained exactly as described before, using various types of experimental data, including water to solvent partitions, gas to solvent partitions, solubility and chromatographic data [51]. Solute descriptors used in the present study are all based on experimental data. There is also commercial software [52] and several published estimation schemes [13,53–56] available for calculating the numerical values of solute descriptors from molecular structural information if one is unable to find the necessary partition, solubility and/or chromatographic data.

Table 3
Intercorrelation matrix, in R^2, for solute descriptors in Eq. (10)

	E	**S**	**A**	**L**
E	1.000			
S	0.466	1.000		
A	0.091	0.007	1.000	
L	0.054	0.018	0.110	1.000

3. Results and discussion

We have assembled in Table 1 values of $\Delta H_{\text{Solv,BE}}$ for 68 gaseous solutes dissolved in dibutyl ether covering a reasonably wide range of compound type and descriptor values. Preliminary analysis of the experimental data yielded a correlation equation

$$\begin{aligned}\Delta H_{\text{Solv,BE}}(\text{kJ/mol}) = {} & -7.205(0.787) + 6.190(1.386)\mathbf{E} \\ & - 7.583(1.179)\mathbf{S} - 36.482(1.595)\mathbf{A} \\ & + 4.093(1.108)\mathbf{B} - 9.263(0.198)\mathbf{L} \end{aligned} \quad (9)$$

(with $N = 68$, S.D. = 1.564, $R^2 = 0.976$, $R^2_{\text{adj}} = 0.974$ $F = 495.9$) that had relatively small numerical value for the *b*-coefficient. The coefficient for the **B** solute descriptor was set equal to zero as would be expected for the transfer of a gaseous solute into an ether solvent having no acidic H-bond character, and the final regression analyses performed to give

$$\begin{aligned}\Delta H_{\text{Solv,BE}}(\text{kJ/mol}) = {} & -6.366(0.826) + 3.943(1.365)\mathbf{E} \\ & - 5.105(1.062)\mathbf{S} - 33.970(1.581)\mathbf{A} \\ & - 9.325(0.217)\mathbf{L} \end{aligned} \quad (10)$$

(with $N = 68$, S.D. = 1.882, $R^2 = 0.970$, $R^2_{\text{adj}} = 0.968$, $F = 513.5$)

$$\begin{aligned}\Delta H_{\text{Solv,BE}}(\text{kJ/mol}) = {} & 0.324(1.199) - 6.480(1.748)\mathbf{E} \\ & - 14.644(1.534)\mathbf{S} - 37.094(2.047)\mathbf{A} \\ & + 4.354(1.418)\mathbf{B} - 32.989(0.913)\mathbf{V} \end{aligned} \quad (11)$$

(with $N = 68$, S.D. = 2.003, $R^2 = 0.960$, $R^2_{\text{adj}} = 0.957$, $F = 298.0$)

There was very little decrease in descriptive ability resulting from setting the coefficient equal to zero. The standard deviation increased very slightly from S.D. = 1.564 (Eq. (9)) to 1.882 (Eq. (10)), which is less than the estimated uncertainty associated with the experimental data. The intercorrelation matrices, in R^2, between the descriptors used in Eqs. (10) and (11) are given in Tables 3 and 4, respectively. Intercorrelations between most of the descriptors are negligible, and even the largest intercorrelation between **E** and **S**, 0.466 (Eq. (10)) and 0.546 (Eq. (11)), is not too significant. The intercorrelation between the **E** and **S** solute descriptors has been noted in earlier papers [57–60]. All regression analyses were performed using SPSS statistical software [61].

Table 4
Intercorrelation matrix, in R^2, for solute descriptors in Eq. (11)

	E	**S**	**A**	**B**	**V**
E	1.000				
S	0.546	1.000			
A	0.148	0.113	1.000		
B	0.213	0.303	0.181	1.000	
V	0.000	0.035	0.075	0.006	1.000

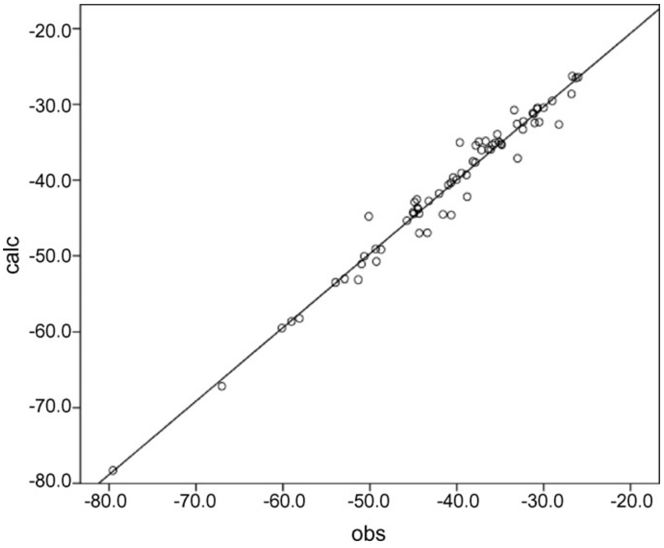

Fig. 1. A plot of the calculated values of $\Delta H_{\text{Solv,BE}}$ based on Eq. (10) against the observed values.

Both Eqs. (10) and (11) are statistically very good with standard deviations of 1.882 and 2.003 kJ/mol for a data set that covers a range of about 53 kJ/mol. See Fig. 1 for a plot of the calculated values of $\Delta H_{\text{Solv,BE}}$ based on Eq. (10) against the observed values. Equation (10) is slightly the better equation statistically, and from a thermodynamic standpoint Eq. (10) is the enthalpic temperature derivative of the Abraham model's gas-to-condensed phase transfer equation. The Abraham solute descriptors are taken to be independent of temperature [62,63]. Equation (11) might be more useful in some predictive applications in instances where the **L**-descriptor is not known. Equation (11) uses the McGowan volume, **V**-descriptor, which is easily calculable from the individual atomic sizes and numbers of bonds in the molecule [13].

We are aware of one group method and an earlier application of the Abraham model for estimating enthalpies of solvation in dibutyl ether. Bernazzani et al. [14] predicted the $\Delta H_{\text{Solv,BE}}$ values of 59 compounds in dibutyl ether to within a standard deviation of 1.59 kJ/mol using 22 structural fragment values deduced by a multiple least-squares regression analysis of the entire data set. The authors' second method, in which the CH_2 group value was preassigned an average of the increments of the enthalpies of solvation in homologous series of alkanes, ethers, 1-alkanols, ketones, amines and chloroalkanes, gave a slightly larger deviation of 3.78 kJ/mol. Our method of Eq. (10) is quite comparable and predicts the enthalpies of solvation in dibutyl ether to within a standard deviation of 1.882 kJ/mol. Bernazzani et al. [64] described the $\Delta H_{\text{Solv,BE}}$ values of 28 compounds in dibutyl ether using the Abraham equation and molecular descriptors. The authors obtained a standard deviation of 0.97 kJ/mol for their correlation equation for the 28 compounds that spanned at most a range of 50 kJ/mol.

The enthalpy of solvation database for dibutyl ether contains only 68 solutes. It would be difficult to obtain a good training set correlation by using only half of the experimental values. To assess the predictive ability of Eq. (10) the parent data points were divided into three subsets (A, B, and C) as follows: the 1st, 4th, 7th, etc. data points comprise the first subset (A); the 2nd, 5th, 8th, etc. data points comprise the second subset (B); and the 3rd, 6th, 9th, etc. data points comprise the third subset (C). Three training sets were prepared as combinations of two subsets (A and B), (A and C), and (B and C). For each training set, a correlation was derived:

Training Set (A and B)

$$\Delta H_{\text{Solv,BE}}(\text{kJ/mol}) = -6.270(0.780) + 4.044(1.351)\mathbf{E} - 4.377(1.044)\mathbf{S} - 34.356(1.525)\mathbf{A} - 9.414(0.201)\mathbf{L} \quad (12)$$

with $N = 46$, S.D. = 1.394, $R^2 = 0.984$, $R^2_{\text{adj}} = 0.983$, $F = 633.3$

Training Set (A and C)

$$\Delta H_{\text{Solv,BE}}(\text{kJ/mol}) = -6.374(1.094) + 4.079(1.761)\mathbf{E} - 5.982(1.418)\mathbf{S} - 33.789(1.982)\mathbf{A} - 9.275(0.310)\mathbf{L} \quad (13)$$

with $N = 45$, S.D. = 1.748, $R^2 = 0.966$, $R^2_{\text{adj}} = 0.963$, $F = 286.4$

Training Set (B and C)

$$\Delta H_{\text{Solv,BE}}(\text{kJ/mol}) = -6.571(1.290) + 3.729(1.952)\mathbf{E} - 5.201(1.488)\mathbf{S} - 33.328(2.562)\mathbf{A} - 9.241(0.315)\mathbf{L} \quad (14)$$

with $N = 45$, S.D. = 1.975, $R^2 = 0.956$, $R^2_{\text{adj}} = 0.952$, $F = 218.5$.

Each validation computation gave a training set correlation equation having coefficients not too different from that obtained from the parent 68 compound database. The training set equations were then used to predict $\Delta H_{\text{Solv,BE}}$ values for the compounds in the respective test sets (A, B and C). Computations on the three test sets yielded: standard deviations of S.D. = 1.680 (Test set C), S.D. = 1.734 (Test set B) and S.D. = 1.155 (Test set A); Average Absolute Errors of AAE = 1.618 (Test set C), AAE = 1.323 (Test set B) and AAE = 0.706 (Test set A); and Average Errors of AE = −0.302 (Test set C), AE = 0.462 (Test set B) and AE = −0.108 (Test set A). There is therefore very little bias in the predictions based on Eqs. (12)–(14).

In Table 2 are collected values of the molar enthalpies of solvation of 79 compounds in ethyl acetate. Regression analysis of the experimental $\Delta H_{\text{Solv,EA}}$ data in accordance with the Abraham model yielded

$$\Delta H_{\text{Solv,EA}}(\text{kJ/mol}) = -7.063(0.705) + 4.671(0.963)\mathbf{E} - 15.141(1.084)\mathbf{S} - 28.763(1.423)\mathbf{A} - 7.691(0.169)\mathbf{L} \quad (15)$$

with $N = 79$, S.D. = 2.156, $R^2 = 0.977$, $R^2_{\text{adj}} = 0.976$, $F = 797.7$

$$\begin{aligned}\Delta H_{\text{Solv,EA}}(\text{kJ/mol}) = {} & 0.679(0.909) - 4.403(1.146)\mathbf{E} \\ & - 20.424(1.504)\mathbf{S} - 32.125(1.543)\mathbf{A} \\ & - 1.299(1.256)\mathbf{B} - 28.598(0.670)\mathbf{V}\end{aligned} \tag{16}$$

with $N = 79$, S.D. = 2.279, $R^2 = 0.975$, $R^2_{\text{adj}} = 0.973$, $F = 561.3$

Again, the b·**B** term is eliminated from Eq. (15) because ethyl acetate has no acidic hydrogen-bonding capability. The b·**B** term was retained in Eqs. (11) and (16) as there is no theoretical reason that we know of for setting the term equal to zero. There is little intercorrelation between the descriptors in Eqs. (15) and (16); the maximum intercorrelation is $R^2 = 0.524$ (Eq. (15)) and $R^2 = 0.664$ (Eq. (16)) between **E** and **S**.

In the original Abraham model for gas-to-condensed phase transfer the equation coefficients encode chemical information about the condensed solubilizing solvent media [1,7]. For the water-to-organic solvent transfer expression the coefficients represent differences in the properties of the organic solvent relative to those of water. While we have used the Abraham expression for water-to-organic solvent transfer to correlate enthalpies of solvation for solutes dissolved in dibutyl ether (Eq. (11)) and in ethyl acetate (Eq. (16)) we realize that the equation coefficients have lost their original significance. Equations (11) and (16) are not the 1/*T* derivative of the Abraham model water-to-organic solvent log *P* correlation. Both Eqs. (15) and (16) are statistically very good with standard deviations of 2.156 and 2.279 kJ/mol for a data set that covers a range of about 76 kJ/mol. Fig. 2 compares the calculated values of $\Delta H_{\text{Solv,EA}}$ based on Eq. (15) against the observed values. To our knowledge, there has been no previous attempt to correlate $\Delta H_{\text{Solv,EA}}$ data.

To assess the predictive ability of Eq. (15), the 79 data points were divided into three subsets (A, B, C) as before: the 1st, 4th, 7th, etc. data points comprise the first subset (A); the 2nd, 5th, 8th, etc. data points comprise the second subset (B); and the 3rd, 6th, 9th, etc. data points comprise the third subset (C). Three training sets were prepared as combinations of two subsets (A and B), (A and C), and (B and C). For each training set, a correlation was derived:

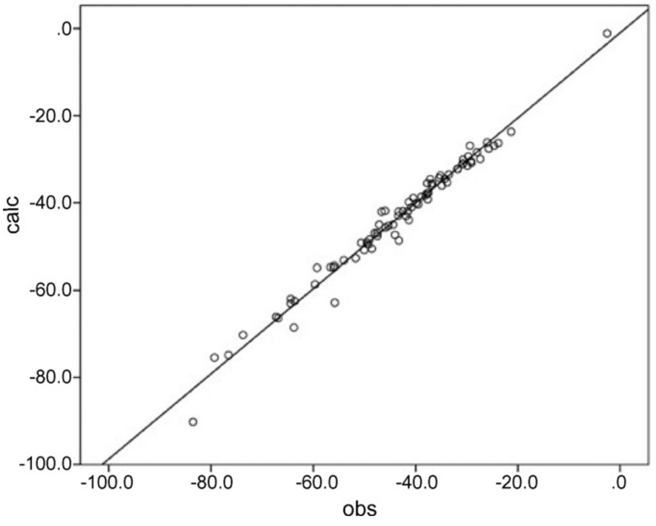

Fig. 2. A plot of the calculated values of $\Delta H_{\text{Solv,EA}}$ based on Eq. (15) against the observed values.

Training Set (A and B)

$$\begin{aligned}\Delta H_{\text{Solv,EA}}(\text{kJ/mol}) = {} & -7.893(0.747) + 5.262(1.233)\mathbf{E} \\ & - 15.641(1.240)\mathbf{S} - 26.597(1.567)\mathbf{A} \\ & - 7.481(0.188)\mathbf{L}\end{aligned} \tag{17}$$

(with $N = 53$, S.D. = 1.914, $R^2 = 0.980$, $R^2_{\text{adj}} = 0.979$, $F = 596.5$)

Training Set (A and C)

$$\begin{aligned}\Delta H_{\text{Solv,EA}}(\text{kJ/mol}) = {} & -5.967(1.013) + 5.638(1.196)\mathbf{E} \\ & - 16.147(1.431)\mathbf{S} - 31.228(1.842)\mathbf{A} \\ & - 7.919(0.227)\mathbf{L}\end{aligned} \tag{18}$$

(with $N = 53$, S.D. = 2.211, $R^2 = 0.974$, $R^2_{\text{adj}} = 0.972$, $F = 445.5$)

Training Set (B and C)

$$\begin{aligned}\Delta H_{\text{Solv,EA}}(\text{kJ/mol}) = {} & -6.945(0.858) + 3.826(1.154)\mathbf{E} \\ & - 14.322(1.330)\mathbf{S} - 28.692(1.812)\mathbf{A} \\ & - 7.714(0.207)\mathbf{L}\end{aligned} \tag{19}$$

(with $N = 52$, S.D. = 2.201, $R^2 = 0.980$, $R^2_{\text{adj}} = 0.978$, $F = 574.0$)

Each validation computation gave a training set correlation equation having coefficients not too different from that obtained from the parent 79 compound database. The training set equations were then used to predict $\Delta H_{\text{Solv,EA}}$ values for the compounds in the respective test sets (A, B and C). Computations on the three test sets yielded: standard deviations of S.D. = 2.757 (Test set C), S.D. = 2.309 (Test set B) and S.D. = 2.121 (Test set A); Average Absolute Errors of AAE = 2.189 (Test set C), AAE = 1.508 (Test set B) and AAE = 1.623 (Test set A); and Average Errors of AE = −0.360 (Test set C), AE = 0.445 (Test set B) and AE = −0.427 (Test set A). There is therefore very little bias in the predictions based on Eqs. (17)–(19).

More than 40 different water-to-organic solvent, gas-to-organic solvent, gas-to-humic acid and/or gas-to-folvic acid partition systems have been reported in the published chemical and environmental literature based on the Abraham model as modified by Goss [8–12]. While we personally prefer to use the Abraham model for the reasons discussed previously [65]; however, we do recognize that the Goss modification is now being used to correlate experimental partition coefficient and sorption data. Our past computations [65,66] have shown that there is very little difference in the descriptive ability of the Abraham model and Goss modified Abraham model when applied to partition coefficient data. The descriptive abilities of the two models have not been compared using other solute properties.

The single comparison involving $\Delta H_{\text{Solv,W}}$ data used different methodologies and datasets.

Goss [67] proposed an indirect method for estimating $\Delta H_{\text{Solv,W}}$ on the basis of Eq. (5). The author used the experimental gas-to-water partition coefficients at 298 K reported by Abraham et al. [68], along with the enthalpies of solvation compiled by Kühne et al. [69] in order to calculate the gas-to-water partition coefficients at several temperatures between 273 and 318 K. A separate $\log K_{\text{w}}$ (where K_{w} is the gas-to-water partition coefficient) was developed for each temperature studied based on Eq. (5). The derived $\log K_{\text{w}}$ correlations were then used to generate predicted $\log K_{\text{w}}$ values at each temperature, which were then plotted versus $1/T$. Enthalpies of solvation were back-calculated from the slopes of the resulting $\log K_{\text{w}}$ versus $1/T$ curves for each of the 217 compounds studied. No statistical information was given in the paper comparing the back-calculated and observed $\Delta H_{\text{Solv,W}}$ values; however, the graphical comparison the author presented showed deviations as large as 10–15 kJ/mol for many of the 217 compounds studied. Eq. (1), derived by Mintz et al. [1] provided a more accurate prediction of $\Delta H_{\text{Solv,W}}$ than did the indirect method of Goss. The experimental $\Delta H_{\text{Solv,W}}$ database used in generating Eq. (1) was not the same as the database used by Goss. Mintz et al. [1] constructed their $\Delta H_{\text{Solv,W}}$ database from published experimental data in the temperature range of 283–318 K. Experimental data outside of this temperature were excluded from consideration. Enthalpies of solvation are temperature dependent and the authors did not want to introduce large errors in the database by including experimental data far removed from 298 K. The Kühne et al. [69] database used by Goss covered a temperature range of from 0 to 100 °C. An assessment of the descriptive ability of the Abraham model versus the Goss modified Abraham model needs to be performed using identical $\Delta H_{\text{Solv,W}}$ databases.

As part of the current study mathematical correlations were developed for both dibutyl ether

$$\Delta H_{\text{Solv,BE}}(\text{kJ/mol}) = -4.350(1.111) - 8.983(1.551)\mathbf{S} - 35.970(1.604)\mathbf{A} + 3.530(1.095)\mathbf{B} - 5.997(0.798)\mathbf{L} - 11.730(2.913)\mathbf{V} \quad (20)$$

(with $N = 68$, S.D. = 1.602, $R^2 = 0.974$, $R^2_{\text{adj}} = 0.972$, $F = 472.9$) and ethyl acetate

$$\Delta H_{\text{Solv,EA}}(\text{kJ/mol}) = -3.476(1.087) - 16.482(1.660)\mathbf{S} - 30.388(1.399)\mathbf{A} - 1.551(1.082)\mathbf{B} - 4.330(0.732)\mathbf{L} - 12.601(2.786)\mathbf{V} \quad (21)$$

(with $N = 79$, S.D. = 2.055, $R^2 = 0.979$, $R^2_{\text{adj}} = 0.978$, $F = 694.0$) based on the Goss modified Abraham model. Both equations provide very good descriptions of the observed enthalpy of solvation data (see Fig. 3 for a plot of $\Delta H_{\text{Solv,BE}}$ based on Eq. (20) versus experimental values), and are comparable in descriptive ability to Eqs. (10) and (15) based on the Abraham model. The slightly lower standard deviations for Eqs. (20) and (21) were likely the result of the one additional curve-fit coefficient. The F-test takes into account the number of descriptors and hence the F-statistics for Eqs. (20) and (21) (472.9 and 694.0) are not quite as good as those for Eqs. (10) and (15) (513.5 and 797.7).

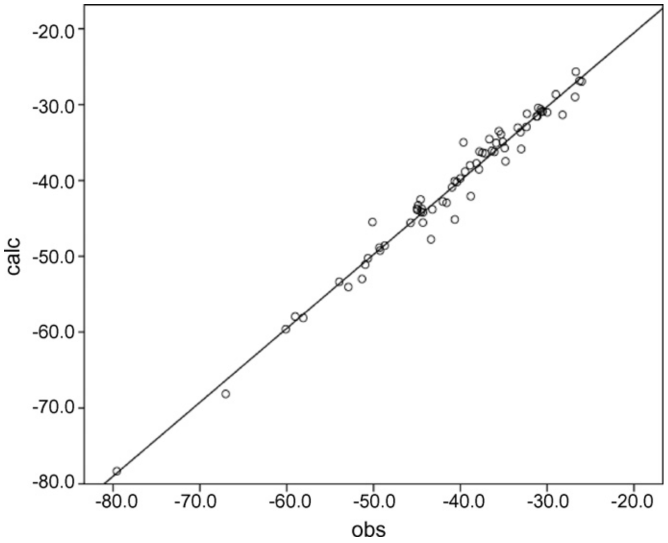

Fig. 3. A plot of the calculated values of $\Delta H_{\text{Solv,BE}}$ based on Eq. (20) against the observed values.

The b·**B** term was retained in Eqs. (20) and (21) as there is no theoretical reason that we know of for setting the term equal to zero. When the Abraham model was developed each of the five terms represented a different type of molecular interaction as discussed above. The existing numerical values of our solute descriptors were determined based on the defined five-term separation of molecular interactions. Goss eliminated the e·**E** term that involved solute–solvent interactions arising through the presence of polarizable electrons in the solute in favor of adding a second cavity effect. The l·**L** and v·**V** terms are both cavity “size” terms measuring the endoergic effect of disrupting solvent–solvent interactions. Solute volume/size is well correlated with molar refraction and with polarizability, and the v·**V** and l·**L** terms will also include exoergic solute–solvent effects that arise through solute polarizability. There is no guarantee though that once the e·**E** term is removed that all of its mathematical contribution will end up in the v·**V** and l·**L** terms. Some of the removed polarizable effect may be mathematically distributed to the a·**A** and b·**B** terms. We do not think that this is a problem here as both the a- and b-coefficients of the four alkane solvents (hexane, heptane, hexadecane and cyclohexane) and two aromatic hydrocarbon solvents (benzene and toluene) have fairly small numerical values.

The correlation matrix, in R^2, between the descriptors used in Eqs. (20) and (21) are given in Tables 5 and 6, respectively. Examination of the numerical entries in Tables 5 and 6 reveals that in the Goss modified version of the Abraham model the solute descriptors are more highly intercorrelated, with R^2 values as large as $R^2 = 0.937$ (Eq. (20)) and $R^2 = 0.953$ (Eq. (21)) between the **L** and **V** solute descriptors. High intercorrelations were also noted between the **L** and **S** (**V** and **S**) solute descrip-

Table 5
Intercorrelation matrix, in R^2, for solute descriptors in Eq. (20)

	S	**A**	**B**	**L**	**V**
S	1.000				
A	0.106	1.000			
B	0.256	0.156	1.000		
L	0.716	0.113	0.157	1.000	
V	0.740	0.158	0.133	0.937	1.000

tors. As noted by two of the Reviewers, intercorrelations of this magnitude between solute descriptors are highly undesirable in the development of QSPR correlations. If intercorrelated solute parameters are used, there could be many different sets of solvent parameters that fit the experimental data. If this were to happen, then the numerical values of solvent parameters obtained from intercorrelation lose their physical meaning. This is one of the reasons that the Abraham model uses only **L** or **V** (and not both) in a derived correlation equation. While the Goss modified form of the Abraham model has been used to mathematically correlate water-to-organic solvent, gas-to-humic acid and/or gas-to-folvic acid partition systems no one has critically evaluated the equation coefficients to determine if the calculated values are reasonable given the types of molecular interactions that are believed to be present in the various partition systems studied by the Goss modified Abraham model. Such a determination will require Goss modified Abraham model equation coefficients for several types of process, and for a several different organic solvents.

Equation coefficients and the associated statistical information are given in Table 7 for the Goss modified Abraham model for organic and gaseous solutes dissolved in hexane, heptane, hexadecane, cyclohexane, benzene, toluene, carbon tetrachloride, chloroform, 1,2-dichloroethane, methanol, ethanol, 1-butanol, 1-octanol, propylene carbonate, dimethyl sulfoxide and water. The ΔH_{Solv} databases used in deriving the correlations are given in our earlier publications [1–7]. Examination of the numerical entries reveals that the Goss modified version of the Abraham model correlated the ΔH_{Solv} data to within an overall average standard deviation of 2.29 kJ/mol for water and the 17 organic solvents studied. The standard deviations are comparable to those noted previously for the Abraham model correlations that were derived from the same ΔH_{Solv} data sets. We defer discussion of the numerical values of the equation coefficients until such time that ΔH_{Solv} correlations become available for more of the other polar organic solvents such as *N*,*N*-dimethylformamide and acetonitrile.

Table 6
Intercorrelation matrix, in R^2, for solute descriptors in Eq. (21)

	S	**A**	**B**	**L**	**V**
S	1.000				
A	0.001	1.000			
B	0.317	0.008	1.000		
L	0.776	0.021	0.166	1.000	
V	0.757	0.049	0.157	0.953	1.000

Table 7
Equation coefficients for ΔH_{Solv} correlations based on the Goss modified Abraham model

Solvent	c	s	a	b	l	v	*N*	S.D.	R^2
Hexane	−3.164 (0.680)	−2.191 (1.039)	0.755 (1.270)	0.692 (0.749)	−6.746 (0.425)	−10.808 (1.751)	118	1.663	0.989
Heptane	−3.783 (0.697)	−2.312 (1.037)	−1.224 (1.508)	1.179 (0.840)	−6.341 (0.437)	−11.276 (1.780)	134	1.687	0.987
Hexadecane	−2.968 (0.710)	−3.204 (1.049)	−1.505 (1.126)	2.579 (0.834)	−6.786 (0.467)	−10.856 (1.908)	102	1.601	0.988
Cyclohexane	−5.059 (0.538)	0.974 (0.830)	−0.510 (0.939)	−2.007 (0.690)	−7.631 (0.352)	−5.284 (1.386)	201	1.828	0.985
Benzene	−2.880 (0.740)	−11.713 (1.206)	−8.224 (1.721)	−5.085 (0.898)	−6.880 (0.498)	−5.892 (1.963)	174	2.212	0.985
Toluene	−3.660 (0.923)	−12.984 (1.411)	−6.298 (1.769)	−5.119 (0.968)	−6.877 (0.612)	−5.623 (2.524)	108	2.229	0.986
Carbon tetrachloride	3.714 (0.708)	−6.522 (0.985)	−1.553 (1.093)	−6.982 (0.730)	−6.451 (0.408)	−9.325 (1.763)	177	2.054	0.984
Chloroform	−2.043 (0.990)	−17.802 (1.516)	−4.536 (1.734)	−17.429 (0.956)	−1.996 (0.685)	−23.780 (2.594)	100	2.108	0.982
1,2-Dichloroethane	−0.163 (1.018)	−19.040 (1.488)	−9.828 (1.944)	−8.196 (1.035)	−4.556 (0.628)	−12.097 (2.400)	88	1.844	0.979
Methanol	−7.172 (0.806)	−2.449 (1.214)	−37.225 (1.199)	−14.370 (0.867)	−8.646 (0.522)	3.292 (2.040)	188	2.739	0.982
Ethanol	−6.300 (1.080)	−1.327 (1.490)	−11.042 (1.236)	−48.528 (1.755)	−8.113 (0.600)	−0.517 (2.554)	111	2.531	0.982
1-Butanol	−5.557 (1.068)	−2.183 (1.712)	−52.603 (2.039)	−3.689 (1.180)	−7.091 (0.716)	−6.087 (2.919)	103	2.274	0.986
1-Octanol	−6.672 (0.741)	6.044 (1.104)	−53.656 (2.373)	−9.190 (1.120)	−9.663 (0.336)	1.566 (1.397)	138	2.591	0.989
Propylene carbonate	−2.267 (1.252)	−16.484 (1.830)	−20.377 (2.216)	−10.693 (1.316)	−4.823 (0.811)	−7.524 (3.250)	107	2.543	0.964
Dimethyl sulfoxide	−2.390 (0.958)	−19.041 (1.510)	−47.799 (1.781)	−5.521 (1.000)	−6.189 (0.706)	−0.746 (2.609)	150	2.791	0.968
Water	−8.414 (1.007)	0.732 (1.285)	−33.558 (1.470)	−43.462 (0.958)	−1.403 (0.579)	−17.313 (2.466)	368	4.739	0.941

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