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Enthalpy of solvation correlations for organic solutes and gases dissolved in 1-propanol and tetrahydrofuran

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ABSTRACT

Data have been assembled from the published literature on the enthalpies of solvation for 103 organic vapors and gaseous solutes in 1-propanol and for 86 gaseous compounds in tetrahydrofuran. It is shown that an Abraham solvation equation with five descriptors can be used to correlate the experimental solvation enthalpies to within standard deviations of 2.35 kJ/mole and 2.10 kJ/mole for 1-propanol and tetrahydrofuran, respectively. The derived correlations provide very accurate mathematical descriptions of the measured enthalpy of solvation data at 298 K, which in the case of 1-propanol span a range of 119 kJ/mole. Division of the experimental values into a training set and a test set shows that there is no bias in predictions, and that the predictive capability of the correlations is better than 3.5 kJ/mole.

1. Introduction

Linear free energy relationship (LFER) models represent a consolidated computational method to mathematically correlate thermodynamic transfer properties and permeabilities of chemical compounds to molecular features (called molecular descriptors) that range in type from topological and structural indices to electronic and quantum-chemical properties. Representative properties that have been correlated with LFER models include sorption of organic compounds on polydimethylsiloxane coated fibers [1–3], chromatographic retention times of organic compounds and drug molecules on immobilized artificial membrane chromatographic columns [4–6], solute partitioning between water and an immiscible (or partly miscible) organic solvent [7–10], solute partitioning between two partly miscible organic solvents [11–14], drug distribution from blood to the various body organs [15–20], permeability of organic compounds through human skin from aqueous solution [21], brain permeation of neutral molecules and ionic species [22], and enthalpies of solvation of organic vapors and gases in both water [23] and in organic solvent media [23–32]. 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 correlate experimental enthalpies of solvation of organic vapors and gases in water, $\Delta H_{\mathrm{solv,w}}$, [23]:

$$\begin{aligned}\Delta H_{\mathrm{solv,w}}\ \ (\mathrm{kJ/mol}) = {} & -13.310(0.457) + 9.910(0.814)\ \ \mathbf{E}\\ & +2.836(0.807)\ \ \mathbf{S} - 32.010(1.102)\ \ \mathbf{A}\\ & -41.816(0.781)\ \ \mathbf{B} - 6.354(0.200)\ \ \mathbf{L}\\ & (N = 368,\quad \mathrm{SD} = 3.68,\quad R^2 = 0.964,\\ & F = 1950.5)\end{aligned} \tag{1}$$

$$\begin{aligned}\Delta H_{\mathrm{solv,w}}\ \ (\mathrm{kJ/mol}) = {} & -6.952(0.651) + 1.415(0.770)\ \ \mathbf{E}\\ & +2.859(0.855)\ \ \mathbf{S} - 34.086(1.225)\ \ \mathbf{A}\\ & -42.868(0.850)\ \ \mathbf{B} - 22.720(0.800)\ \ \mathbf{V}\\ & (N = 369,\quad \mathrm{SD} = 4.04,\quad R^2 = 0.959,\quad F = 1688.2)\end{aligned} \tag{2}$$

and in four alkanes (hexane [27], heptane [29], hexadecane [29] and cyclohexane [29]), in two aromatic hydrocarbons (benzene [29] and toluene [31]), in three chloroalkanes (trichloromethane [30], tetrachloromethane [31] and 1,2-dichloroethane [30]), in five alcohols (methanol [26], ethanol [26], 1-butanol [26], 1-octanol [23] and *tert*-butanol [25]), and in seven other organic solvents (acetone [24], propylene carbonate [32], dimethyl sulfoxide [32], dibutyl ether [28], ethyl acetate [28], acetonitrile [24] and *N*,*N*-dimethylformamide [25]). In total Abraham model, ΔH_{solv}

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correlations have been reported for total of 22 different organic solvents. Expressions have also been developed for predicting the enthalpies of solvation of organic vapors and gases into ionic liquid solvents based on the ionic-specific equation coefficient [33] and group contribution [34] versions of the Abraham model.

Each term in Eqs. (1) and (2) represents a different type of solute–solvent interaction contributing to the solute transfer process. The independent variables are solute descriptors, which are defined as follows: **E** denotes the solute excess molar refraction that reflects the solute's ability to interact with the surrounding solvent molecules through π- and lone-electron pairs, **S** is the solute dipolarity/polarizability parameter, **A** and **B** are measures of the solute's hydrogen-bond acidity and basicity, **V** is the McGowan volume of the solute in units of $(\text{dm}^3\ \text{mol}^{-1})/100$, and **L** is the logarithm of the solute's gas phase dimensionless Ostwald partition coefficient into hexadecane at 298 K. The first four descriptors can be regarded as measures of the tendency of the given compounds to undergo various solute–solvent interactions. The latter two descriptors, **V** and **L**, are both measures of solute size, and so will be measures of the solvent cavity term that will accommodate the dissolved solute. General dispersions are also related to solute size; hence both **V** and **L** will also describe the general solute–solvent interactions.

Numerical values of the six equation coefficients in Eqs. (1) and (2) are determined by multiple linear regression analyses of experimental ΔH_{solv} data for a series of organic solutes and gases in the solvent under consideration. The statistics of the derived correlation are the number of experimental values in the regressed database (N), the standard deviation (SD), the squared correlation coefficient (R^2) and the Fisher F-statistic. Standard uncertainties in the calculated equation coefficients are given in parenthesis immediately after the respective coefficient.

During the past two years we have been updating several of our existing gas-to-organic solvent partition coefficient, K, and water-to-organic solvent partition coefficient, P, correlations [35–38], and introducing additional terms into the equation ($\text{j}^+\cdot\mathbf{J}^+$ and $\text{j}^-\cdot\mathbf{J}^-$) that enable the prediction of P values of neutral molecules, ions and ionic species at 298 K [39–41]. Previously log P the correlations had been limited in applicability to just neutral molecules. As part of these studies we have determined solute descriptors for several simple ions and several classes of organic ionic species (carboxylate anions, substituted phenoxide anions, substituted pryridinium cations and protonated amines). The descriptors for anions and cations are **E**, **S**, **A**, **B**, and are exactly on the same scale as for neutral molecules, together with an additional descriptor, $\mathbf{J}^-$, for anions and an additional descriptor, $\mathbf{J}^+$, for cations.

Our published Abraham model partition coefficient correlations have for the most part pertained to 298 K. Manufacturing and biological processes are not restricted to 298 K, and there is a growing need to estimate gas-to-organic solvent and water-to-organic solvent partition coefficients at other temperatures as well. From a thermodynamic standpoint, ΔH_{Solv} data can be used to estimate the gas-to-condensed phase partition coefficient, K,

$$\log\ K(\text{at}\ T) - \log\ K(\text{at}\ 298.15\ \text{K}) = \frac{-\Delta H_{\text{Solv}}}{2.303R}\left(\frac{1}{T} - \frac{1}{298.15}\right) \tag{3}$$

and the water-to-organic solvent partition coefficient, P,

$$\log\ P(\text{at}\,T) - \log\ P(\text{at}\ 298.15\ \text{K}) = \frac{-\Delta H_{\text{trans}}}{2.303R}\left(\frac{1}{T} - \frac{1}{298.15}\right) \tag{4}$$

at other temperatures from measured partition coefficient data at 298.15 K and the solute's enthalpy of solvation, ΔH_{Solv}, or enthalpy of transfer, ΔH_{trans}, between the two condensed phases. The enthalpy of transfer needed in Eq. (4) is defined as

$$\Delta H_{\text{trans}} = \Delta H_{\text{Solv,Org}} - \Delta H_{\text{Solv,W}} \tag{5}$$

the difference in the enthalpy of solvation of the solute in the specified organic solvent minus its enthalpy of solvation in water. The above equations assume zero heat capacity changes. The 22 ΔH_{solv} correlations that we have developed thus far allow us to extrapolate log P and log K values measured at 298 K to other temperatures. Eventually we hope to develop mathematical expressions for predicting enthalpies of solvation in most (if not all) of the more than 70 organic solvents for which we have log K and log P correlations. The present study concerns developing a ΔH_{solv} correlation for solutes dissolved in 1-propanol and in tetrahydrofuran. The log K and log P correlations for both organic solvents were recently updated [35,38].

2. Data sets and solute descriptors

A search of the published chemical literature found a large number of papers [42–140] that reported experimental partial molar enthalpies of solution, ΔH_{soln}, of liquid solutes in 1-propanol and tetrahydrofuran, or excess molar enthalpies of binary mixtures containing either 1-propanol or tetrahydrofuran. The ΔH_{soln} data for the liquid solutes were determined by either direct calorimetric methods or calculated based on the temperature dependence of the measured infinite dilution activity coefficient data. Calorimetric data was also found for the dissolution of a few gases in tetrahydrofuran [141,142], and for five crystalline organic solutes, ethylene carbonate [143], benzamide [144], benzoic acid [145], 1-bromoadamantane [146] and 1-adamantanol [147], in 1-propanol. Enthalpies of solution of several gas molecules [148–155], anthracene [156], acenaphthene [157], adipic acid [158], succinic acid [159] and sebacic acid [160] were calculated from the variation of mole fraction solubility with temperature. The ΔH_{soln} values were converted to gas-to-organic solvent enthalpies of transfer by

$$\text{Liquid solutes}: \quad \Delta H_{\text{Solv}} = \Delta H_{\text{Soln}} - \Delta H_{\text{Vap,298K}} \tag{6}$$

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

subtracting the solute's standard molar enthalpy of vaporization [161,162], $\Delta H_{\text{Vap,298 K}}$, or standard molar enthalpy of sublimation [162,163], $\Delta H_{\text{Sub,298 K}}$, at 298.15 K.

We eliminated from consideration all experimental data that pertained to temperatures outside 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. 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 aforementioned criteria, 103 molar enthalpies of solvation in 1-propanol and 86 molar enthalpies of solvation in tetrahydrofuran were selected for regression analysis. The experimental $\Delta H_{\text{Solv,PrOH}}$ and $\Delta H_{\text{Solv,THF}}$ values are listed in Tables 1 and 2 along with the values of the solute descriptors of the compounds considered in the present study. The tabulated solute descriptors are of experimental origin and came from our solute descriptor database, which now contains values for more than 5000 different organic and organometallic compounds. Large tabulations of solute descriptors are available in several earlier publications [23,165,166].

The characteristic McGowan volume, **V**, is calculated from the individual atomic sizes and numbers of bonds in the molecule [164]. For liquid solutes, the excess molar refraction descriptor, **E**, is obtained from the liquid refractive index [167]. In the case of

Table 1
Values of the gas-to-1-propanol solvation enthalpy in kJ/mole at 298 K, $\Delta H_{\mathrm{solv,PrOH}}$, for 103 solutes, together with the solute descriptors.

Solute	**E**	**S**	**A**	**B**	**L**	**V**	ΔH_{solv}	Refs.
Methane	0.000	0.000	0.000	0.000	−0.323	0.2495	−2.09	[149]
Ethane	0.000	0.000	0.000	0.000	0.492	0.3904	−10.33	[149]
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	−18.60	[148]
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	−20.79	[148]
Butane	0.000	0.000	0.000	0.000	1.615	0.6722	−22.10	[148]
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	−25.39	[76]
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	−33.76	[149]
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	−38.45	[70,86]
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	−43.75	[49]
Decane	0.000	0.000	0.000	0.000	4.686	1.5176	−47.35	[47,50]
Dodecane	0.000	0.000	0.000	0.000	5.696	1.7994	−58.09	[47]
2,3-Dimethylbutane	0.000	0.000	0.000	0.000	2.495	0.9540	−27.86	[46]
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.2358	−33.37	[46]
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	−31.14	[53]
Cyclooctane	0.413	0.100	0.000	0.000	4.329	1.1272	−40.98	[77]
1-Propene	0.100	0.080	0.000	0.070	0.946	0.4883	−18.75	[148]
1-Butene	0.100	0.080	0.000	0.070	1.491	0.6292	−19.78	[148]
cis 2-Butene	0.140	0.080	0.000	0.050	1.737	0.6292	−21.55	[147]
trans-2-Butene	0.126	0.080	0.000	0.050	1.664	0.6292	−21.39	[148]
2-Methyl-1-propene	0.120	0.080	0.000	0.080	1.579	0.6292	−21.67	[148]
1-Hexene	0.078	0.080	0.000	0.070	2.572	0.9110	−29.10	[42]
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.0519	−34.00	[42]
1,3-Butadiene	0.320	0.230	0.000	0.100	1.543	0.5862	−20.93	[148]
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	−37.50	[97]
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	−42.20	[71]
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	−47.50	ΔH_{vap}
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	−52.19	[71]
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	−56.81	[71]
Hexan-1-ol	0.210	0.420	0.370	0.480	3.610	1.0127	−60.48	[61]
Octan-1-ol	0.199	0.420	0.370	0.480	4.619	1.2950	−70.07	[59,71]
Decan-1-ol	0.191	0.420	0.370	0.480	5.628	1.5763	−80.00	[60]
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.5900	−45.52	[95]
Benzene	0.610	0.520	0.000	0.140	2.786	0.7176	−31.77	[81]
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	−35.98	[57]
1,4-Dimethylbenzene	0.613	0.520	0.000	0.160	3.839	0.9982	−40.50	[85]
Difluoromethane	−0.320	0.490	0.060	0.050	0.040	0.2489	−9.41	[155]
Trifluoromethane	−0.430	0.180	0.110	0.030	−0.274	0.3026	−12.50	[155]
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.7391	−32.88	[66,67,139]
Chloroethane	0.227	0.400	0.000	0.100	1.678	0.5128	−23.50	[147]
2-Chloro-2-methylpropane	0.142	0.300	0.000	0.030	2.273	0.7946	−27.32	[56]
2-Chloro-2-methylbutane	0.171	0.270	0.000	0.150	2.858	0.9355	−32.93	[56]
2-Chloro-2-methylpentane	0.207	0.390	0.000	0.130	3.520	1.0764	−37.62	[56]
Trichloroethene	0.520	0.370	0.080	0.030	2.997	0.7146	−33.94	[72]
2-Methyl-2-bromopropane	0.305	0.290	0.000	0.070	2.609	0.8472	−29.81	[73,88]
2-Methyl-2-bromobutane	0.343	0.400	0.000	0.150	3.400	0.9881	−35.55	[88]
2-Methyl-2-iodopropane	0.589	0.350	0.000	0.190	3.439	0.9304	−33.37	[73]
1-Bromoadamantane	1.070	0.900	0.000	0.200	6.130	1.3668	−56.01	[145]
Acetone	0.179	0.700	0.040	0.490	1.696	0.5470	−25.00	[82]
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	−28.93	[78]
Dimethyl ether	0.000	0.270	0.000	0.410	1.285	0.4491	−18.30	[147]
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.7309	−26.10	[66]
Diisopropyl ether	−0.060	0.160	0.000	0.580	2.530	1.0127	−32.46	[43,87]
Dibutyl ether	0.000	0.250	0.000	0.450	3.924	1.2950	−43.13	[62]
Butyl methyl ether	0.045	0.250	0.000	0.440	2.658	0.8718	−31.09	[63]
Methyl *tert*-butyl ether	0.024	0.210	0.000	0.590	2.380	0.8718	−28.64	[43,80,84]
Methyl *tert*-amyl ether	0.050	0.210	0.000	0.600	2.916	1.0127	−34.40	[43]
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	−28.97	[87]
Tetrahydropyran	0.275	0.470	0.000	0.550	3.057	0.7672	−34.44	[74,84]
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	−30.79	[44,54]
15-Crown-5	0.410	1.200	0.000	1.750	6.779	1.7025	−70.22	[90]
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162	−53.89	[79]
Argon	0.000	0.000	0.000	0.000	−0.688	0.1900	−1.67	[149]
Xenon	0.000	0.000	0.000	0.000	0.378	0.3290	−9.62	[150]
Nitrogen	0.000	0.000	0.000	0.000	−0.978	0.2222	1.17	[149]
Carbon monoxide	0.000	0.000	0.000	0.040	−0.836	0.2220	−1.72	[149]
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	−9.75	[154]
Oxygen	0.000	0.000	0.000	0.000	−0.723	0.1830	0.50	[149]
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	−29.88	[54]
Propyl acetate	0.092	0.600	0.000	0.450	2.819	0.8875	−33.81	[89]
Butyronitrile	0.180	0.900	0.000	0.360	2.548	0.6860	−31.80	[83]
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538	−44.40	[48,51]
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	−39.49	[64]
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237	−29.67	[44,68]
4-Methylpyridine	0.630	0.820	0.000	0.540	3.640	0.8162	−46.80	[52]
1,3-Dichlorobenzene	0.847	0.730	0.000	0.020	4.410	0.9612	−45.66	[75]

Table 1 (*Continued*)

Solute	**E**	**S**	**A**	**B**	**L**	**V**	ΔH_{solv}	Refs.
1,3-Dimethoxybenzene	0.816	1.010	0.000	0.450	5.022	1.1160	−52.05	[66]
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	−40.07	[58]
1,2-Dimethoxyethane	0.116	0.670	0.000	0.680	2.654	0.7896	−33.60	[54]
1,2-Diethoxyethane	0.008	0.730	0.000	0.790	3.310	1.0714	−40.00	[66]
Tetramethylsilicon	−0.057	0.080	0.000	0.000	1.812	0.9179	−23.00	[55]
Tetramethyltin	0.324	0.110	0.000	0.100	2.651	1.0431	−30.46	[149]
Benzo-15-crown-5	1.055	1.940	0.000	1.590	9.403	2.0285	−82.42	[90]
Tributylamine	0.051	0.150	0.000	0.790	5.983	1.8992	−66.20	[51]
Carbon tetrafluoride	−0.580	−0.260	0.000	0.000	−0.817	0.3203	−1.12	[151]
Sucinnic acid	0.370	1.320	1.030	0.710	3.951	0.8210	−95.70	[159]
Adipic acid	0.350	1.210	1.130	0.760	4.474	1.1028	−105.90	[158]
Sebacic acid	0.350	1.360	1.120	0.870	6.920	1.6664	−118.05	[160]
1,3-Diaminopropane	0.446	0.610	0.430	1.140	2.852	0.7309	−69.50	[91]
3,6,9-Trioxoundecane	0.040	0.870	0.000	1.200	4.815	1.4111	−51.40	[45]
Digylme	0.113	0.760	0.000	1.170	3.920	1.1301	−42.63	[65]
2,2,2-Trifluoroethanol	0.015	0.600	0.570	0.250	1.224	0.5022	−48.33	[94]
N-Methylformamide	0.405	1.360	0.400	0.550	2.863	0.5059	−51.21	[96]
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	−72.34	[156]
Fluoromethane	0.070	0.350	0.000	0.090	0.057	0.2672	−8.12	[152]
Trimethylphosphate	0.113	1.360	0.000	0.930	3.850	0.9707	−40.50	[93]
Tributyl phosphate	−0.100	0.110	0.000	1.260	7.539	2.2390	−79.71	[92]
Ethylene carbonate	0.381	1.250	0.000	0.580	2.670	0.5558	−31.70	[143]
Benzaldehyde	0.820	1.000	0.000	0.390	4.008	0.8730	−44.16	[69]
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586	−57.97	[157]
1-Adamantanol	0.940	0.900	0.310	0.660	5.634	1.2505	−74.59	[146]
Quinoline	1.268	0.970	0.000	0.540	5.457	1.0443	−58.65	[140]
Benzamide	0.990	1.500	0.490	0.670	5.767	0.9728	−81.53	[144]
Benzoic acid	0.730	0.900	0.590	0.400	4.510	0.9317	−74.77	[144]

solid solutes, one either estimates a hypothetical liquid refractive index using any of several available methods, or one can calculate **E** directly through the addition of fragments or substructures. Numerical values of the three remaining descriptors, **S**, **A** and **B**, are determined through regression analysis using available organic solvent/water partition coefficients, chromatographic retention data, solubilities and infinite dilution activity coefficients as described elsewhere [168–172]. If one is unable to locate sufficient experimental data for performing the fore-mentioned regression analysis, commercial software [173] is available for estimating the molecular solute descriptors from the structure of the compound. Several correlations [174,175] have been reported for calculating the Abraham solute descriptors from the more structure-based, topological-based and/or quantum-based descriptors used in other QSAR and LFER treatments. Moreover, van Noort et al. [176] published an Abraham model correlation for estimating the **L** solute descriptor

$$\mathbf{L} = -0.882 + 1.183\ \mathbf{E} + 0.839\ \mathbf{S} + 0.454\ \mathbf{A} + 0.157\ \mathbf{B} + 3.505\ \mathbf{V}$$
$$(N = 4785,\quad \text{SD} = 0.31,\quad R^2 = 0.992,\quad F = 115279) \qquad (8)$$

from known values of **E, S, A, B** and **V**. The authors cited a personnel communication from Dr. Abraham as the source of Eq. (8).

3. Results and discussion

We have assembled in Table 1 values of $\Delta H_{\text{Solv,PrOH}}$ for 103 organic vapors and gases dissolved in 1-propanol covering a reasonably wide range of compound type and descriptor value. Analysis of the experimental data yielded the following two Abraham model correlation equations:

$$\Delta H_{\text{Solv,PrOH}}\ (\text{kJ/mole}) = -8.713(0.462) - 2.593(1.086)\ \mathbf{E} + 5.190(1.113)\ \mathbf{S} - 53.042(1.210)\ \mathbf{A} - 7.852(1.094)\ \mathbf{B} - 8.108(0.193)\ \mathbf{L}$$
$$(\text{with}\ N = 101,\quad \text{SD} = 2.41,\quad R^2 = 0.989,\quad F = 1678) \qquad (9)$$

$$\Delta H_{\text{Solv,PrOH}}\ (\text{kJ/mole}) = -0.114(0.801) - 12.428(1.272)\ \mathbf{E} + 2.052(1.495)\ \mathbf{S} - 55.258(1.571)\ \mathbf{A} - 7.964(1.426)\ \mathbf{B} - 30.202(0.955)\ \mathbf{V}$$
$$(\text{with}\ N{=}103,\quad \text{SD} = 3.13,\quad R^2 = 0.981,\quad F = 986.2) \qquad (10)$$

All regression analyses were performed using Version 17 of the SPSS statistical software. There is little intercorrelation between the descriptors in Eqs. (9) and (10). Both correlations provide a good statistical fit of the observed data with standard deviations of 2.41 and 3.13 kJ/mole for a data set that covers a range of about 119.0 kJ/mole. See Fig. 1 for a plot of the calculated values $\Delta H_{\text{Solv,PrOH}}$ based on Eq. (9) against the observed values. Eq. (9) is the better equation statistically, and from a thermodynamic standpoint Eq. (9) is the enthalpic derivative of the Abraham model's gas-to-condensed phase transfer equation. Eq. (10) might be more useful in some predictive applications in instances where the **L**-descriptor is not known. Eq. (10) uses the McGowan volume, **V**-descriptor, which is easily calculable from the individual atomic sizes and numbers of bonds in the molecule [164]. To our knowledge, Eqs. (9) and (10) are the first expressions that allow one to predict the enthalpy of solvation of gaseous solutes in 1-propanol.

In order to assess the predictive ability of Eq. (9) we divided the 103 data points into a training set and a test set by allowing the SPSS software to randomly select half of the experimental points. The selected data points became the training set and the compounds that were left served as the test set. Analysis of the experimental data in the training set gave

$$\Delta H_{\text{Solv,PrOH}}\ (\text{kJ/mole}) = -8.712(0.723) - 7.321(1.665)\ \mathbf{E} + 7.590(1.889)\ \mathbf{S} - 53.653(1.871)\ \mathbf{A} - 8.950(1.690)\ \mathbf{B} - 8.159(0.269)\ \mathbf{L}$$
$$(\text{with}\ N = 52,\quad \text{SD} = 2.70,\quad R^2 = 0.988,\quad F = 767.4) \qquad (11)$$

Table 2
Values of the gas-to-tetrahydrofuran solvation enthalpy in kJ/mole at 298 K, $\Delta H_{solv,THF}$, for 86 solutes, together with the solute descriptors.

Solute	**E**	**S**	**A**	**B**	**L**	**V**	ΔH_{solv}	Refs.
Methane	0.000	0.000	0.000	0.000	−0.323	0.2495	−3.02	[153]
Ethane	0.000	0.000	0.000	0.000	0.492	0.3904	−13.74	[153]
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	−16.69	[153]
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	−28.39	[128]
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	−33.38	[127]
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	−37.55	[120,124]
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	−42.14	[120]
Decane	0.000	0.000	0.000	0.000	4.686	1.5176	−46.13	[101]
Dodecane	0.000	0.000	0.000	0.000	5.696	1.7994	−56.53	[123]
Tetradecane	0.000	0.000	0.000	0.000	6.705	2.0812	−64.36	[101]
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.9540	−27.28	[124]
2,2-Dimethylbutane	0.000	0.000	0.000	0.000	2.352	0.9540	−24.83	[129]
2,3-Dimethylbutane	0.000	0.000	0.000	0.000	2.495	0.9540	−26.21	[129]
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	−29.39	[112,113]
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.9863	−32.87	[112,127]
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.2358	−32.90	[122,127]
Ethene	0.107	0.100	0.000	0.070	0.289	0.3474	−11.42	[153]
1-Hexene	0.078	0.080	0.000	0.070	2.572	0.9110	−29.18	[130]
Cyclohexene	0.395	0.200	0.000	0.100	3.021	0.8025	−32.33	[137]
Dichloromethane	0.387	0.570	0.100	0.050	2.019	0.4943	−34.17	[104]
Trichloromethane	0.425	0.490	0.150	0.020	2.480	0.6167	−39.62	[99,103]
Tetrachloromethane	0.458	0.380	0.000	0.000	2.823	0.7391	−35.72	[105]
1-Chlorobutane	0.210	0.400	0.000	0.100	2.722	0.7946	−34.46	[117]
1,1,2,2-Tetrachloroethane	0.595	0.760	0.160	0.120	3.803	0.8800	−57.03	[132,133]
Chlorocyclohexane	0.448	0.480	0.000	0.100	3.832	0.9678	−43.10	[112]
Trichloroethene	0.524	0.370	0.080	0.030	2.997	0.7146	−39.69	[134]
Tetrachloroethene	0.639	0.440	0.000	0.000	3.584	0.8370	−40.66	[134]
Dipropyl ether	0.008	0.250	0.000	0.450	2.954	1.0127	−34.60	[118]
Diisopropyl ether	-0.060	0.160	0.000	0.580	2.530	1.0127	−31.40	[125]
Dibutyl ether	0.000	0.250	0.000	0.450	3.924	1.2945	−44.14	[118]
Methyl tert-butyl ether	0.024	0.110	0.000	0.630	2.380	0.8718	−29.97	[119]
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	−32.00	ΔH_{vap}
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	−33.90	[98]
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	−37.99	[98]
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.7309	−47.86	[117]
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.5900	−38.23	[74]
1-Hexanol	0.210	0.420	0.370	0.480	3.610	1.0170	−56.98	[87]
1-Heptanol	0.211	0.420	0.370	0.480	4.115	1.1536	−61.76	[87]
1-Octanol	0.199	0.420	0.370	0.480	4.619	1.2950	−65.59	[87]
1-Nonanol	0.193	0.420	0.370	0.480	5.120	1.4354	−71.16	[87]
1-Decanol	0.191	0.420	0.370	0.480	5.628	1.5763	−75.31	[87]
2-Methoxyethanol	0.269	0.500	0.300	0.840	2.490	0.6487	−42.80	[138]
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	−33.70	[121]
Butyronitrile	0.180	0.900	0.000	0.360	2.548	0.6860	−39.66	[116]
Benzene	0.610	0.520	0.000	0.140	2.786	0.7176	−35.24	[102]
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	−38.77	[102]
1,4-Dimethylbenzene	0.613	0.520	0.000	0.160	3.839	0.9982	−43.23	[114]
1,2,4-Trimethylbenzene	0.677	0.560	0.000	0.190	4.441	1.1391	−48.70	[107]
Anisole	0.710	0.750	0.000	0.290	3.890	0.9160	−48.93	[117]
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	−43.77	[109,100]
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.7341	−37.60	[126]
Nitrobenzene	0.871	1.110	0.000	0.280	4.557	0.8906	−57.72	[66]
Benzyl chloride	0.821	0.860	0.000	0.140	4.353	0.9797	−52.75	[100]
Pyrrole	0.613	0.730	0.410	0.290	2.865	0.5770	−53.26	[102]
N-Methylpyrrole	0.559	0.790	0.000	0.310	2.923	0.7180	−41.56	[102,106]
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162	−62.86	[66]
Helium	0.000	0.000	0.000	0.000	−1.741	0.0680	8.12	[153]
Neon	0.000	0.000	0.000	0.000	−1.575	0.0850	7.01	[153]
Argon	0.000	0.000	0.000	0.000	−0.688	0.1900	−0.04	[153]
Krypton	0.000	0.000	0.000	0.000	−0.211	0.2460	−3.39	[153]
Xenon	0.000	0.000	0.000	0.000	0.378	0.3290	−8.85	[153]
Hydrogen	0.000	0.000	0.000	0.000	−1.200	0.1086	4.48	[153]
Deuterium	0.000	0.000	0.000	0.000	−1.200	0.1100	6.01	[153]
Nitrogen	0.000	0.000	0.000	0.000	−0.978	0.2222	1.32	[153]
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	−17.02	[141]
Carbon tetrafluoride	−0.580	−0.260	0.000	0.000	−0.817	0.3203	−0.02	[153]
Sulfur hexafluoride	−0.600	−0.200	0.000	0.000	−0.120	0.4643	4.83	[153]
Pyridine	0.631	0.840	0.000	0.520	3.022	0.6753	−39.60	[131]
2-Methylpyridine	0.598	0.750	0.000	0.580	3.422	0.8162	−42.00	[131]
3-Methylpyridine	0.631	0.810	0.000	0.540	3.631	0.8162	−44.00	[131]
4-Methylpyridine	0.630	0.820	0.000	0.540	3.640	0.8162	−44.30	[131]
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538	−33.30	[48]
Hexafluorobenzene	0.088	0.560	0.000	0.010	2.345	0.8226	−35.50	[136]
Sulfur dioxide	0.370	0.660	0.280	0.100	0.778	0.3465	−39.30	[142]
15-Crown-5	0.410	1.200	0.000	1.750	6.779	1.7025	−78.89	[135]

Table 2 (*Continued*)

Solute	**E**	**S**	**A**	**B**	**L**	**V**	ΔH_{solv}	Refs.
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751	−71.00	[117]
4-Fluorophenol	0.670	0.970	0.630	0.230	3.844	0.7928	−74.61	[117]
1-Chloronaphthalene	1.417	1.000	0.000	0.140	5.856	1.2078	−68.35	[110]
1-Methylnaphthalene	1.337	0.940	0.000	0.220	5.802	1.2260	−60.24	[111]
Dimethyl carbonate	0.142	0.540	0.000	0.570	2.328	0.6644	−36.90	[108]
Diethyl carbonate	0.060	0.580	0.000	0.530	3.412	0.9462	−42.28	[108]
Diethylamine	0.154	0.300	0.080	0.690	2.395	0.7720	−33.27	[115]
Dipropylamine	0.124	0.300	0.080	0.690	3.351	1.0538	−40.13	[115]
Hexanoic acid	0.174	0.630	0.620	0.440	3.697	1.0284	−71.78	[66]
Octanoic acid	0.150	0.640	0.620	0.450	4.680	1.3102	−82.88	[66]
4-Fluoroanisole	0.571	0.740	0.000	0.280	3.904	0.9337	−51.84	[117]

There is very little difference in the equation coefficients for the full dataset and the training dataset correlations, thus showing that the training set of compounds is a representative sample of the total data set. The training set equation was then used to predict $\Delta H_{\mathrm{Solv,PrOH}}$ values for the 51 compounds in the test set. For the predicted and experimental values, we find SD = 2.26, AAE (average absolute error) = 1.81 and AE (average error) = −0.10 kJ/mole. There is therefore very little bias in using Eq. (11) with AE equal to −0.10 kJ/mole. The training set and test set analyses were performed two more times with similar results. Training and test validations were also performed for Eq. (10). To conserve journal space, we give only the test set results. The derived training set correlation for Eq. (10) predicted the 51 experimental $\Delta H_{\mathrm{Solv,PrOH}}$ values in the test set to within a SD = 3.14, AAE = 2.44 and AE = 0.01 kJ/mole Again, there is very little bias in the predictions using Eq. (10) with AE equal to 0.01 kJ/mole. An error/uncertainty of ±2 kJ/mole in the enthalpy of solvation results in an error of slightly less than 0.04 log units in extrapolating a log *K* value measured at 298.15 K to a temperature of 313.15. This level of predictive error will be sufficient for most practical chemical and engineering applications.

In Table 2 are collected values of the enthalpies of solvation of 86 gaseous solutes in tetrahydrofuran. Preliminary analysis of the experimental $\Delta H_{\mathrm{Solv,THF}}$ data yielded correlation equations having very small *b* coefficients, would be expected from the molecular structure considerations. Tetrahydrofuran does not have an acidic hydrogen. The *b*-coefficients were set equal to zero, and the final regression analyses performed to give:

$$\begin{aligned}\Delta H_{\mathrm{Solv,THF}}\ (\mathrm{kJ/mole}) &= -6.040(0.437) + 3.640(1.223)\ \mathbf{E}\\ &\quad -14.478(1.252)\ \mathbf{S} - 40.652(1.455)\ \mathbf{A}\\ &\quad -8.537(0.150)\ \mathbf{L}\\ (\text{with}\ \ N = 86,\ \ \mathrm{SD} &= 2.10,\ \ R^2 = 0.990,\ \ F = 1997) \qquad (12)\end{aligned}$$

$$\begin{aligned}\Delta H_{\mathrm{Solv,THF}}\ (\mathrm{kJ/mole}) &= 4.777(0.894) - 6.642(1.146)\ \mathbf{E}\\ &\quad -23.110(1.502)\ \mathbf{S} - 43.222(1.764)\ \mathbf{A}\\ &\quad -33.683(0.724)\ \mathbf{V}\\ (\text{with}\ \ N = 86,\ \ \mathrm{SD} &= 2.55,\ \ R^2 = 0.985,\ \ F = 1346) \qquad (13)\end{aligned}$$

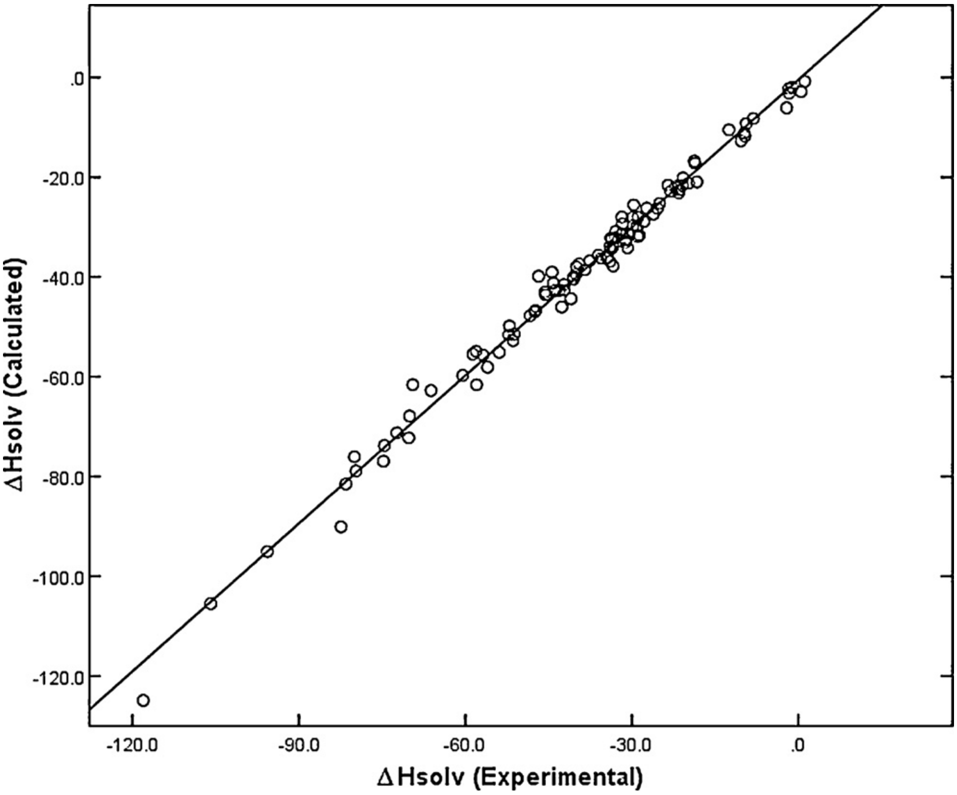

Fig. 1. A plot of the calculated values of $\Delta H_{\mathrm{Solv,PrOH}}$ based on Eq. (9) against the observed values.

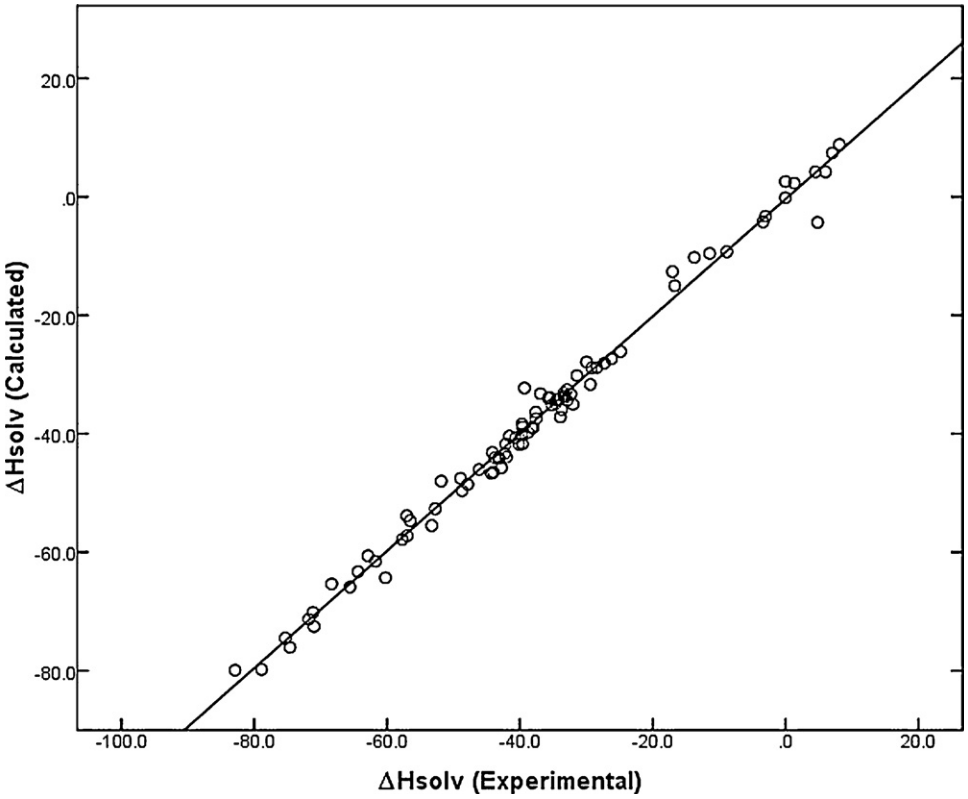

Fig. 2. A plot of the calculated values of $\Delta H_{\text{Solv,THF}}$ based on Eq. (12) against the observed values.

Both Eqs. (12) and (13) are statistically very good with standard deviations of 2.10 and 2.55 kJ/mole for a dataset that covers an approximate range of 91.0 kJ/mole. Both equations were validated through training and test set analyses. Fig. 2 compares the calculated values of $\Delta H_{\text{Solv,THF}}$ based on Eq. (12) against the observed data. To our knowledge there has been no previous attempt to correlate enthalpies of solvation for gaseous solutes in tetrahydrofuran.

The predictive ability of Eq. (13) was assessed as before by allowing the SPSS software to randomly divide the 86 experimental data points into training and test sets. Analyses of the experimental data in the training set gave

$$\begin{aligned}\Delta H_{\text{Solv,THF}}\ \text{(kJ/mole)} &= -6.549(0.596) + 5.800(1.797)\ \mathbf{E}\\ &\quad -15.407(1.876)\ \mathbf{S} - 42.258(2.357)\ \mathbf{A}\\ &\quad -8.448(0.186)\ \mathbf{L}\\ &(\text{with}\ \ N = 43,\ \ \text{SD} = 1.94,\ \ R^2 = 0.990,\ \ F = 942.6) \qquad (14)\end{aligned}$$

There is very little difference in the equation coefficients for the full dataset and the training dataset correlations, thus showing that the training set of compounds is a representative sample of the total data set. The training set equation was then used to predict $\Delta H_{\text{Solv,THF}}$ values for the 43 compounds in the test set. For the predicted and experimental values, we find SD = 2.44, AAE = 1.97 and AE = 0.35 kJ/mole. There is therefore very little bias in using Eq. (14) with AE equal to 0.35 kJ/mole. The training set and test set analyses were performed two more times with similar results. Training and test validations were also performed for Eq. (13). To conserve journal space, we give only the test set results. The derived training set correlation for Eq. (13) predicted the 43 experimental $\Delta H_{\text{Solv,THF}}$ values in the test set to within a SD = 3.03, AAE = 2.26 and AE = 0.54 kJ/mole. Again, there is very little bias in the predictions using Eq. (13) with AE equal to 0.54 kJ/mole.

The correlations presented in this study further document the applicability of the Abraham solvation parameter model to describe enthalpies of solvation for organic vapors and gaseous solutes dissolved in organic solvents. The derived ΔH_{Solv} correlations for 1-propanol and tetrahydrofuran will allow one to extrapolate gas-to-PrOH(or THF) and water-to-PrOH(or THF) measured at 298.15 K to other temperatures. Not all manufacturing applications occur at 298.15 K, and there is a growing need in the chemical industry to predict solute transfer and partition properties at other temperatures as well.

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