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Enthalpy of solvation correlations for gaseous solutes dissolved in dimethyl sulfoxide and propylene carbonate based on the Abraham model

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Abstract

Data have been assembled from the published literature on the enthalpies of solvation for more than 100 compounds in dimethyl sulfoxide and propylene carbonate. 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 2.80 and 2.61 kJ/mol for dimethyl sulfoxide and propylene carbonate, respectively. The derived correlations provide very accurate mathematical descriptions of the measured enthalpy of solvation data at 298 K, which in the case of dimethyl sulfoxide span a range of about 92 kJ/mol. 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 3.6 kJ/mol.

Keywords: Enthalpy of solvation; Enthalpy of transfer; Mathematical correlation; Partition coefficient; Solvation parameter model

1. Introduction

The thermodynamic properties of molecules in various chemical and biological processes are greatly influenced by molecular interactions between the molecule and its solubilizing media. Such interactions may be either non-specific or specific in nature. Non-specific interactions are described by a random distribution of molecules throughout the entire solution. Specific interactions, on the other hand, are generally much stronger and often result in a specific geometric orientation of one molecule with respect to an adjacent molecule. Even in systems known to contain specific interactions, the need to properly account for non-specific interactions has been long recognized.

In previous studies [1–10] we have used the Abraham solvation parameter model to describe mathematically the various solute–solvent interactions found in a wide range of different chemical and biological systems. We have reported partition coefficient correlations (both water-to-organic solvent and gas-to-organic solvent) for more than 50 common organic solvents. Our published correlations have for the most part pertained to 298.15 K. Manufacturing and biological processes are not restricted to 298.15 K, and there is a need to estimate partitioning properties in water and in organic solvents at other temperatures as well. From a thermodynamic standpoint, the gas-to-condensed phase partition coefficient, K, and water-to-organic solvent partition coefficient, P, can be estimated:

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

and

$$\log P\,(\text{at }T) - \log P\,(\text{at }298.15\,\text{K}) = \frac{-\Delta H_{\text{trans}}}{R}\left(\frac{1}{T} - \frac{1}{298.15}\right) \quad (2)$$

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. (2) is defined as

$$\Delta H_{\text{trans}} = \Delta H_{\text{Solv,Org}} - \Delta H_{\text{Solv,W}} \quad (3)$$

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.

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Mintz et al. [11] recently developed the correlation equations for enthalpies of solvation in water, $\Delta H_{\text{Solv,W}}$:

$$\begin{aligned}\Delta H_{\text{Solv,W}}\ (\text{kJ/mol}) &= -13.310(0.457) + 9.910(0.814)E + 2.836(0.807)S \\ &\quad - 32.010(1.102)A - 41.816(0.781)B - 6.354(0.200)L \\ &\quad (\text{with } N = 368,\ \text{S.D.} = 3.68, \\ &\quad R^2 = 0.964,\ R^2_{\text{adj}} = 0.964,\ F = 1950.5)\end{aligned} \tag{4}$$

$$\begin{aligned}\Delta H_{\text{Solv,W}}\ (\text{kJ/mol}) &= -6.952(0.651) + 1.415(0.770)E - 2.859(0.855)S \\ &\quad - 34.086(1.225)A - 42.686(0.850)B - 22.720(0.800)V \\ &\quad (\text{with } N = 369,\ \text{S.D.} = 4.04, \\ &\quad R^2 = 0.959,\ R^2_{\text{adj}} = 0.958,\ F = 1688.2)\end{aligned} \tag{5}$$

based on the Abraham model. 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. (4) and (5) are as follows: E and S refer to the excess molar refraction and dipolarity/polarizability descriptors of the solute, respectively, A and B are the solute overall or summation 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 298.15 K. The first four descriptors can be regarded as measures of the tendency of the given solute to undergo various solute–solvent interactions. The 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 dispersion interactions are also related to solute size, hence, both V and L will also describe the general solute–solvent interactions. The regression coefficients and constants (c, e, s, a, b, v and l) are obtained by regression analysis of experimental data for a given process (i.e., a given partitioning processes, a given stationary phase and mobile phase combination, *etc.*).

As part of the study, Mintz et al. [11] also reported correlation equations for estimating enthalpies of solvation of organic solutes in 1-octanol. In follow-up studies the authors [12,13] published the corresponding enthalpic equations for solutes dissolved in heptane, hexadecane, cyclohexane, benzene, toluene and carbon tetrachloride. Each of these latter correlations was based on experimental data for a minimum of 100 organic and inorganic solutes. Eventually, we hope to derive mathematical expressions for predicting enthalpies of solvation in most (if not all) of the organic solvents for which we have $\log K$ and $\log P$ correlations. The present study concerns developing ΔH_{Solv} equations for dimethyl sulfoxide and propylene carbonate. We have elected for the present time to correlate only enthalpies of solvation because there is considerably more experimental data available for ΔH_{Solv} than for ΔH_{trans}. To correlate enthalpies of transfer one would need experimental enthalpy of solution data (or ΔH_{Solv} data) for the solute in both water and the organic solvent under consideration. One is more likely to find ΔH_{Solv} in water or the specified organic solvent, than to find both experimental values. Also, enthalpies of solvation allow one to estimate the temperature dependence of partition coefficients of solutes distributed between two immiscible organic solvents. Poole and coworkers [14–16] have recently reported partition coefficient data for neutral compounds between heptane and methanol, *N*,*N*-dimethylformamide, 2,2,2-trifluoroethanol, or 1,1,1,3,3,3-hexafluoro-2-propanol, and between hexane and acetonitrile. The correlations derived in the present study for the enthalpies of solvation in dimethyl sulfoxide and propylene carbonate can be used in conjunction with Eq. (1) and our existing gas-to-organic solvent correlations for dimethyl sulfoxide and propylene carbonate to calculate $\log K$ for the solubility of gases and vapors in both solvents to be carried out for temperatures other than 298 K.

2. Experimental methods

Our search of the chemical literature found a large number of papers [17–83] that reported experimental partial molar 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

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

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

subtracting the solute's standard molar enthalpy of vaporization [84], $\Delta H_{\text{Vap,298 K}}$, or standard molar enthalpy of sublimation [85], $\Delta H_{\text{Sub,298 K}}$, 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 either 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, 150 molar enthalpies of solvation in dimethyl sulfoxide and 107 molar enthalpies of solvation in propylene carbonate were selected for regression analysis. The experimental $\Delta H_{\text{Solv,DMSO}}$ and $\Delta H_{\text{Solv,PC}}$ values are listed in Tables 1 and 2, respectively.

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

Table 1
Values of the gas to dimethyl sulfoxide solvation enthalpy in kJ/mol at 298 K for 150 solutes, together with the solute descriptors

Solute	*E*	*S*	*A*	*B*	*L*	*V*	Exp.	Ref.
Butane	0.000	0.000	0.000	0.000	1.615	0.6722	−12.10	[23]
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	−15.23	[19]
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	−17.61	[78]
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	−21.13	[78]
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	−24.10	[78]
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	−27.66	[78]
Decane	0.000	0.000	0.000	0.000	4.686	1.5176	−30.79	[78]
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	−21.60	[29]
1-Butene	0.100	0.080	0.000	0.070	1.491	0.6292	−15.50	[23]
1-Pentene	0.093	0.080	0.000	0.070	2.047	0.7701	−20.31	[27]
1-Hexene	0.078	0.080	0.000	0.070	2.572	0.9110	−21.51	[27]
1-Octene	0.094	0.080	0.000	0.070	3.568	1.1928	−31.78	[27]
1,3-Butadiene	0.320	0.230	0.000	0.100	1.543	0.5862	−17.00	[23]
1-Octyne	0.155	0.220	0.090	0.100	3.521	1.1498	−37.15	[36]
2-Octyne	0.225	0.300	0.000	0.100	3.850	1.1498	−37.36	[36]
Benzene	0.610	0.520	0.000	0.140	2.786	0.7176	−30.71	[43,46]
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	−34.40	[79]
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	−37.32	[79]
1,3-Dimethylbenzene	0.623	0.520	0.000	0.160	3.839	0.9982	−41.75	[43]
Propylbenzene	0.604	0.500	0.000	0.150	4.230	1.1391	−39.86	[79]
Isopropylbenzene	0.602	0.490	0.000	0.160	4.084	1.1391	−39.66	[33]
Mesitylene	0.649	0.520	0.000	0.190	4.344	1.1391	−39.37	[57]
Butylbenzene	0.600	0.510	0.000	0.150	4.730	1.2800	−42.66	[79]
Pentylbenzene	0.594	0.510	0.000	0.150	5.230	1.4210	−45.44	[79]
Hexylbenzene	0.591	0.500	0.000	0.150	5.720	1.5618	−48.72	[79]
Heptylbenzene	0.577	0.480	0.000	0.150	6.219	1.7027	−52.16	[79]
Octylbenzene	0.579	0.480	0.000	0.150	6.714	1.8436	−53.12	[79]
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854	−53.19	[45]
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3240	−60.96	[43]
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4540	−76.60	[56]
Methylamine	0.250	0.350	0.160	0.580	1.300	0.3493	−26.80	[47]
n-Propylamine	0.225	0.350	0.160	0.610	2.141	0.6311	−30.23	[79]
n-Butylamine	0.224	0.350	0.160	0.610	2.618	0.7720	−33.59	[79]
n-Pentylamine	0.211	0.350	0.160	0.610	3.139	0.9129	−36.48	[79]
n-Hexylamine	0.197	0.350	0.160	0.610	3.655	1.0538	−40.40	[79]
n-Heptylamine	0.197	0.350	0.160	0.610	4.153	1.1947	−43.15	[79]
Acetone	0.179	0.700	0.040	0.490	1.696	0.5470	−29.87	[17]
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	−32.47	[17]
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.8288	−35.49	[27]
2-Hexanone	0.136	0.680	0.000	0.510	3.286	0.9697	−39.80	[56]
2-Heptanone	0.123	0.680	0.000	0.510	3.760	1.1106	−41.00	[17]
4-Heptanone	0.110	0.660	0.000	0.510	3.705	1.1106	−39.83	[17]
2-Octanone	0.108	0.680	0.000	0.510	4.257	1.2515	−43.90	[56]
2-Nonanone	0.119	0.680	0.000	0.510	4.735	1.3924	−47.20	[17]
5-Nonanone	0.103	0.660	0.000	0.510	4.698	1.3924	−44.81	[17]
2,2,4,4-Tetramethyl-3-pentanone	0.099	0.560	0.000	0.520	4.370	1.3924	−35.15	[17]
Cyclohexanone	0.403	0.860	0.000	0.560	3.792	1.0020	−41.84	[17]
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.7309	−21.59	[58]
Dipropyl ether	0.008	0.250	0.000	0.450	2.954	1.0127	−29.59	[48]
Dibutyl ether	0.000	0.250	0.000	0.450	3.924	1.2945	−32.01	[18]
Ethyl propyl ether	0.000	0.250	0.000	0.450	2.493	0.8718	−25.25	[48]
n-Butyl methyl ether	0.045	0.250	0.000	0.440	2.658	0.8718	−25.36	[57]
Methyl heptyl ether	0.048	0.250	0.000	0.450	4.088	1.2945	−36.38	[18]
Methyl *tert*-butyl ether	0.024	0.210	0.000	0.590	2.380	0.8718	−24.23	[58]
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	−27.34	[22]
Tetrahydropyran	0.275	0.470	0.000	0.550	3.057	0.7672	−30.16	[22]
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	−36.63	[22]
1,2-Dimethoxyethane	0.116	0.670	0.000	0.680	2.654	0.7896	−34.73	[22]
1,2-Diethoxyethane	0.008	0.730	0.000	0.790	3.310	1.0714	−39.15	[22]
Furan	0.369	0.510	0.000	0.130	1.913	0.5363	−29.99	[49]
12-Crown-4	0.420	0.990	0.000	1.390	5.135	1.3620	−65.98	[38]
15-Crown-5	0.410	1.200	0.000	1.750	6.779	1.7025	−78.85	[38]
18-Crown-6	0.400	1.340	0.000	2.130	7.919	2.0430	−103.86	[50]
1-Fluorooctane	−0.020	0.350	0.000	0.100	3.850	1.2538	−37.49	[18]

Table 1 (*Continued*)

Solute	*E*	*S*	*A*	*B*	*L*	*V*	Exp.	Ref.
Dichloromethane	0.387	0.570	0.100	0.050	2.019	0.4943	−34.27	[31]
Chloroform	0.425	0.490	0.150	0.020	2.480	0.6167	−36.78	[37]
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.7391	−32.40	[33]
1-Chlorobutane	0.210	0.400	0.000	0.100	2.722	0.7946	−27.68	[39]
1-Chlorooctane	0.191	0.400	0.000	0.090	4.708	1.3580	−39.79	[18]
2-Chloro-2-methylpropane	0.142	0.300	0.000	0.030	2.273	0.7946	−22.72	[39]
1,1,1-Trichloroethane	0.369	0.410	0.000	0.090	2.733	0.7576	−30.03	[32]
1,1,2,2-Tetrachloroethane	0.595	0.760	0.160	0.120	3.803	0.8800	−56.82	[44]
Dibromomethane	0.714	0.690	0.110	0.070	2.886	0.5995	−39.22	[59]
Methyl iodide	0.676	0.430	0.000	0.120	2.106	0.5077	−26.39	[39]
1-Iodobutane	0.628	0.400	0.000	0.150	3.628	0.9304	−33.49	[39]
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.7341	−34.45	[20]
1,2-Difluorobenzene	0.390	0.630	0.000	0.060	2.843	0.7518	−34.93	[21]
1,3-Difluorobenzene	0.374	0.580	0.000	0.060	2.776	0.7518	−34.41	[21]
4-Fluorotoluene	0.488	0.550	0.000	0.140	3.366	0.6750	−36.99	[20]
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	−39.23	[20]
1,2-Dichlorobenzene	0.872	0.780	0.000	0.040	4.518	0.9612	−48.31	[21]
1,3-Dichlorobenzene	0.847	0.730	0.000	0.020	4.410	0.9612	−51.20	[21]
1,4-Dichlorobenzene	0.825	0.750	0.000	0.020	4.435	0.9612	−43.90	[56]
4-Chlorotoluene	0.705	0.740	0.000	0.050	4.205	0.9797	−43.13	[20]
Bromobenzene	0.882	0.730	0.000	0.090	4.041	0.8914	−42.32	[20]
Iodobenzene	1.188	0.820	0.000	0.120	4.502	0.9746	−48.30	[19]
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	−33.24	[80]
Propanenitrile	0.162	0.900	0.020	0.360	2.082	0.5451	−34.57	[80]
1-Butanenitrile	0.188	0.900	0.000	0.360	2.548	0.6860	−36.87	[80]
1-Pentanenitrile	0.177	0.900	0.000	0.360	3.108	0.8269	−41.04	[80]
1-Hexanenitrile	0.166	0.900	0.000	0.360	3.608	0.9678	−43.54	[80]
1-Heptanenitrile	0.159	0.900	0.000	0.360	4.089	1.1087	−46.30	[80]
1-Octanenitrile	0.162	0.900	0.000	0.360	4.585	1.2496	−49.87	[80]
1-Nonanenitrile	0.159	0.900	0.000	0.360	4.970	1.3905	−53.36	[80]
1-Decanenitrile	0.156	0.900	0.000	0.360	5.460	1.5314	−56.98	[80]
1-Undecanenitrile	0.154	0.900	0.000	0.360	5.940	1.6723	−59.66	[80]
1-Dodecanenitrile	0.152	0.900	0.000	0.360	6.460	1.8132	−63.30	[80]
1-Tridecanenitrile	0.150	0.900	0.000	0.360	6.924	1.9541	−66.13	[80]
1-Tetradecanitrile	0.149	0.900	0.000	0.360	7.403	2.0950	−68.94	[80]
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	−39.17	[80]
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	−41.13	[80]
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.5900	−43.76	[80]
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.5900	−41.56	[43]
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.7309	−48.16	[80]
1-Pentanol	0.219	0.420	0.370	0.480	3.106	0.8718	−51.45	[80]
1-Hexanol	0.210	0.420	0.370	0.480	3.610	1.0170	−53.97	[80]
1-Heptanol	0.211	0.420	0.370	0.480	4.115	1.1536	−58.29	[80]
1-Octanol	0.199	0.420	0.370	0.480	4.619	1.2950	−60.25	[18]
1-Nonanol	0.193	0.420	0.370	0.480	5.124	1.4354	−66.92	[80]
1-Decanol	0.191	0.420	0.370	0.480	5.628	1.5763	−68.42	[80]
1-Undecanol	0.181	0.420	0.370	0.480	6.130	1.7173	−70.85	[80]
2-Methyl-2-propanol	0.180	0.300	0.310	0.600	1.963	0.7309	−40.34	[33]
2-Methyl-2-butanol	0.194	0.300	0.310	0.600	2.630	0.8718	−44.52	[58]
Cyclohexanol	0.460	0.540	0.320	0.570	3.758	0.9040	−54.14	[51]
cis-1,2-Cyclohexanediol	0.600	0.860	0.500	0.860	4.203	0.9628	−69.70	[40]
Ethylene glycol	0.404	0.900	0.580	0.780	2.661	0.5078	−69.66	[25]
Propylene glycol	0.373	0.900	0.580	0.800	2.918	0.6487	−66.70	[25]
3-Methylphenol	0.822	0.880	0.570	0.340	4.310	0.9160	−74.56	[58]
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162	−66.48	[53]
N-Methylaniline	0.948	0.940	0.170	0.470	4.494	0.9571	−57.70	[47]
N,*N*-Dimethylaniline	0.957	0.810	0.000	0.410	4.701	1.0980	−49.29	[35]
Dimethyl carbonate	0.142	0.540	0.000	0.570	2.328	0.6644	−34.65	[24]
Diethyl carbonate	0.060	0.580	0.000	0.530	3.412	0.9462	−38.49	[24]
Benzyl alcohol	0.803	0.870	0.330	0.560	4.221	0.9160	−70.30	[26]
2-Phenylethanol	0.811	0.910	0.300	0.640	4.628	1.0569	−70.47	[26]
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057	−30.38	[42]
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	−32.80	[52]
tert-Butyl acetate	0.025	0.540	0.000	0.470	2.802	1.0284	−33.46	[52]
N,*N*-Dimethyl formamide	0.367	1.310	0.000	0.740	3.173	0.6468	−45.64	[42]

Table 1 (*Continued*)

Solute	*E*	*S*	*A*	*B*	*L*	*V*	Exp.	Ref.
N,*N*-Dimethyl acetamide	0.363	1.330	0.000	0.780	3.717	0.7880	−52.29	[42]
Acetophenone	0.818	1.010	0.000	0.480	4.501	1.0140	−51.35	[61]
Pyridine	0.631	0.840	0.000	0.520	3.022	0.6753	−39.00	[35]
2,6-Dimethylpyridine	0.607	0.700	0.000	0.630	3.760	0.9571	−42.60	[54]
Nitrobenzene	0.871	1.110	0.000	0.280	4.557	0.8906	−52.88	[43]
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237	−38.96	[55]
(Trifluoromethy)lbenzene	0.225	0.480	0.000	0.100	2.894	0.9104	−32.68	[57]
Anisole	0.710	0.750	0.000	0.290	3.890	0.9160	−44.27	[57]
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538	−26.30	[34]
Pyrrole	0.613	0.730	0.410	0.290	2.865	0.5770	−54.68	[28]
N-Methylpyrrole	0.559	0.790	0.000	0.310	2.923	0.7180	−40.17	[28]
1,4-Dimethylbenzene	0.613	0.520	0.000	0.160	3.839	0.9982	−37.67	[30]
Diisopropyl ether	−0.060	0.160	0.000	0.580	2.530	1.0127	−26.53	[27]
Ethyl *tert*-butyl ether	−0.020	0.160	0.000	0.600	2.720	1.0127	−27.50	[27]
Methyl *tert*-amyl ether	0.050	0.210	0.000	0.600	2.916	1.0127	−29.07	[27]
Acetaldehyde	0.208	0.670	0.000	0.450	1.230	0.4060	−26.80	[27]
Vinyl acetate	0.223	0.640	0.000	0.430	2.152	0.7040	−30.38	[27]
1-Naphthol	1.520	1.050	0.600	0.370	6.130	1.1441	−90.60	[60]
1-Bromoadamantane	1.070	0.900	0.000	0.200	6.130	1.3668	−50.90	[41]
1-Adamantanol	0.940	0.900	0.310	0.660	5.634	1.2505	−66.00	[41]
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	−12.43	[81]

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 [8]. Solute descriptors used in the present study are all based on experimental data. There is also commercial software [86] and several published estimation schemes [87–90] 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.

3. Results and discussion

We have assembled in Table 1 values of $\Delta H_{\text{Solv,DMSO}}$ for 150 gaseous solutes dissolved in dimethyl sulfoxide covering a reasonably wide range of compound type and descriptor values. Analysis of the experimental data yielded the following correlation equations:

$$\begin{aligned}\Delta H_{\text{Solv,DMSO}}\ (\text{kJ/mol}) &= -2.546(0.703) - 0.329(0.952)E - 18.448(1.139)S \\ &\quad - 47.419(1.653)A - 5.861(1.004)B - 6.380(0.197)L \\ &\quad (\text{with } N = 150,\ \text{S.D.} = 2.80, \\ &\quad R^2 = 0.967,\ R^2_{\text{adj}} = 0.966,\ F = 850.6)\end{aligned} \tag{8}$$

$$\begin{aligned}\Delta H_{\text{Solv,DMSO}}\ (\text{kJ/mol}) &= 2.184(0.845) - 7.233(0.951)E - 24.071(1.175)S \\ &\quad - 50.992(1.744)A - 5.182(1.051)B - 22.301(0.723)V \\ &\quad (\text{with } N = 150,\ \text{S.D.} = 2.92,\ R^2 = 0.965, \\ &\quad R^2_{\text{adj}} = 0.963,\ F = 779.8)\end{aligned} \tag{9}$$

All regression analyses were performed using SPSS statistical software. Both Eqs. (8) and (9) are statistically very good with standard deviations of 2.80 and 2.92 kJ/mol for a data set that covers a range of 91.76 kJ/mol. See Fig. 1 for a plot of the calculated values of $\Delta H_{\text{Solv,DMSO}}$ based on Eq. (8) against the observed values. Eq. (8) is slightly the better equation statistically, and from a thermodynamic standpoint Eq. (8) is the enthalpic temperature derivative of the Abraham model's gas-to-condensed phase transfer equation. Eq. (9) might be more useful in some predictive applications in instances where the *L*-descriptor is not known. Eq. (9) uses the McGowan volume, *V*-descriptor, which is easily calculable from the individual atomic sizes and numbers of bonds in the molecule [91]. To our knowledge, Eqs. (8) and (9) are the first expressions that allow one to predict the enthalpy of solvation of gaseous solutes in dimethyl sulfoxide.

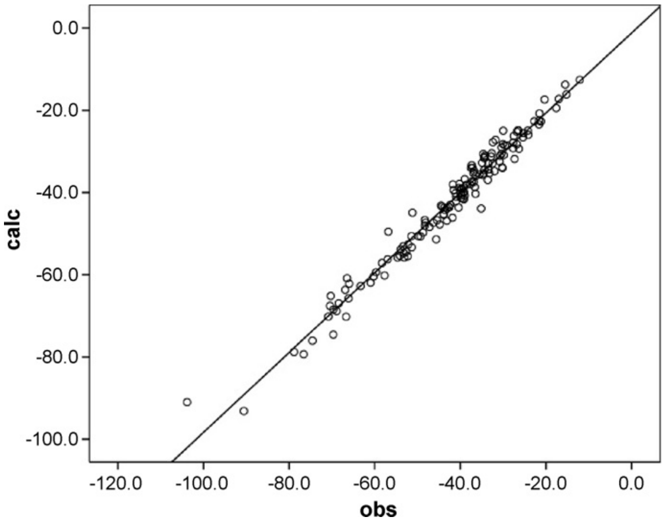

Fig. 1. A plot of the calculated values of $\Delta H_{\text{Solv,DMSO}}$ on Eq. (8) against the observed values.

Table 2
Values of the gas to propylene carbonate solvation enthalpy in kJ/mol at 298 K for 107 solutes, together with the solute descriptors

Solute	*E*	*S*	*A*	*B*	*L*	*V*	Exp.	Ref.
Ethane	0.000	0.000	0.000	0.000	0.492	0.3904	−5.73	[62]
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	−6.44	[62]
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	−9.71	[62]
Butane	0.000	0.000	0.000	0.000	1.615	0.6722	−10.83	[62]
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	−17.57	[62]
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	−21.00	[62]
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	−24.66	[62]
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	−31.41	[27]
Decane	0.000	0.000	0.000	0.000	4.686	1.5176	−37.97	[27]
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	−24.18	[43]
Methylcyclopentane	0.225	0.100	0.000	0.000	2.816	0.8454	−23.14	[27]
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.9863	−26.22	[27]
1-Butene	0.100	0.080	0.000	0.070	1.491	0.6292	−17.60	[23]
1-Hexene	0.078	0.080	0.000	0.070	2.572	0.9110	−24.81	[27]
1-Octene	0.094	0.080	0.000	0.070	3.568	1.1928	−30.56	[27]
Cyclohexene	0.395	0.200	0.000	0.100	3.021	0.8025	−27.01	[27]
1,3-Butadiene	0.320	0.230	0.000	0.100	1.543	0.5862	−19.30	[23]
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057	−32.50	[63]
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	−34.51	[63]
Propyl acetate	0.092	0.600	0.000	0.450	2.819	0.8875	−38.46	[63]
Vinyl acetate	0.223	0.640	0.000	0.430	2.152	0.7040	−34.28	[63]
Butyl acetate	0.071	0.600	0.000	0.450	3.353	1.0284	−41.22	[63]
tert-Butyl acetate	0.025	0.540	0.000	0.470	2.802	1.0284	−35.42	[63]
Isobutyl acetate	0.052	0.570	0.000	0.470	3.161	1.0284	−36.13	[63]
Pentyl acetate	0.067	0.600	0.000	0.450	3.844	1.1693	−45.45	[63]
Hexyl acetate	0.056	0.600	0.000	0.450	4.351	1.3102	−47.36	[63]
Methyl propanoate	0.128	0.600	0.000	0.450	2.431	0.7466	−35.21	[63]
Ethyl propanoate	0.087	0.580	0.000	0.450	2.807	0.8875	−37.79	[63]
Propyl propanoate	0.070	0.560	0.000	0.450	3.338	1.0284	−40.40	[63]
Butyl propanoate	0.058	0.560	0.000	0.470	3.833	1.1693	−46.95	[63]
Methyl butanoate	0.106	0.600	0.000	0.450	2.893	0.8875	−38.08	[63]
Ethyl butanoate	0.068	0.580	0.000	0.450	3.271	1.0284	−39.85	[63]
Propyl butanoate	0.050	0.560	0.000	0.450	3.783	1.1693	−44.43	[63]
Methyl pentanoate	0.108	0.600	0.000	0.450	3.392	1.0284	−40.89	[63]
Ethyl pentanoate	0.049	0.580	0.000	0.450	3.769	1.1693	−43.63	[63]
Ethyl hexanoate	0.043	0.580	0.000	0.450	4.251	1.3102	−48.30	[63]
Ethyl heptanoate	0.027	0.580	0.000	0.450	4.733	1.4511	−47.61	[63]
Ethyl isobutyrate	0.034	0.550	0.000	0.470	3.072	1.0284	−37.63	[63]
Dimethyl carbonate	0.142	0.540	0.000	0.570	2.328	0.6644	−37.49	[65]
Diethyl carbonate	0.060	0.580	0.000	0.530	3.412	0.9462	−42.47	[65]
Acetone	0.179	0.700	0.040	0.490	1.696	0.5470	−30.79	[64]
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	−34.27	[64]
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.8288	−37.60	[27]
2-Hexanone	0.136	0.680	0.000	0.510	3.286	0.9697	−40.78	[64]
2-Octanone	0.108	0.680	0.000	0.510	4.257	1.2515	−47.43	[64]
2-Undecanone	0.101	0.680	0.000	0.510	5.732	1.6740	−59.14	[64]
Cyclohexanone	0.403	0.860	0.000	0.560	3.792	0.8610	−43.77	[64]
2-Methylcyclohexanone	0.372	0.830	0.000	0.560	4.050	1.0020	−45.28	[64]
Anisole	0.710	0.750	0.000	0.290	3.890	0.9160	−45.45	[68]
Phenetole	0.681	0.700	0.000	0.320	4.242	1.0570	−47.61	[68]
Dimethyl sulfoxide	0.522	1.720	0.000	0.970	3.459	0.6126	−51.44	[23]
Benzyl alcohol	0.803	0.870	0.330	0.560	4.221	0.9160	−57.40	[43]
2-Phenylethanol	0.811	0.860	0.310	0.650	4.628	1.0569	−62.37	[69]
3-Phenyl-1-propanol	0.821	0.940	0.310	0.650	5.312	1.1980	−65.00	[69]
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.7309	−25.50	[27]
Diisopropyl ether	−0.060	0.160	0.000	0.580	2.530	1.0127	−28.95	[27]
Methyl *tert*-butyl ether	0.024	0.210	0.000	0.590	2.380	0.8718	−29.09	[27]
Ethyl *tert*-butyl ether	−0.020	0.160	0.000	0.600	2.720	1.0127	−30.73	[27]
Methyl *tert*-amyl ether	0.050	0.210	0.000	0.600	2.916	1.0127	−33.78	[27]
Tetrahydropyran	0.275	0.470	0.000	0.550	3.057	0.7672	−34.33	[70]
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	−31.72	[70]
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	−39.01	[70]
1,3-Dioxolane	0.298	0.510	0.000	0.620	1.830	0.5401	−36.10	[70]
12-Crown-4	0.420	0.990	0.000	1.390	5.135	1.3620	−68.73	[73]

Table 2 (*Continued*)

Solute	*E*	*S*	*A*	*B*	*L*	*V*	Exp.	Ref.
15-Crown-5	0.410	1.200	0.000	1.750	6.779	1.7025	−90.00	[82,83]
18-Crown-6	0.400	1.340	0.000	2.130	7.919	2.0430	−108.86	[71]
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	−31.52	[43]
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	−33.85	[43]
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	−36.80	[43]
Propan-2-ol	0.212	0.360	0.330	0.560	1.764	0.5900	−34.83	[74]
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	−41.31	[43]
2-Butanol	0.217	0.360	0.330	0.560	2.338	0.7309	−38.36	[74]
tert-Butanol	0.180	0.300	0.310	0.600	1.963	0.7309	−36.10	[43]
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	−45.31	[43]
2-Pentanol	0.195	0.360	0.330	0.560	2.840	0.8718	−39.35	[66]
3-Pentanol	0.195	0.360	0.330	0.560	2.860	0.8718	−39.68	[66]
2-Methyl-1-butanol	0.219	0.390	0.370	0.480	3.011	0.8718	−39.90	[43]
2-Methyl-2-butanol	0.194	0.300	0.310	0.600	2.630	0.8718	−38.87	[66]
3-Methyl-1-butanol	0.192	0.390	0.370	0.480	3.011	0.8718	−39.95	[66]
3-Methyl-2-butanol	0.194	0.330	0.330	0.560	2.793	0.8718	−38.84	[66]
Ethan-1,2-diol	0.404	0.900	0.580	0.780	2.661	0.5078	−54.35	[67]
2-Methoxyethanol	0.269	0.500	0.300	0.840	2.490	0.6487	−40.20	[75]
2-Ethoxyethanol	0.237	0.520	0.310	0.810	2.792	0.7896	−42.42	[75]
Benzene	0.610	0.520	0.000	0.140	2.786	0.7176	−32.30	[43]
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	−35.65	[43]
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	−39.19	[43]
Isopropylbenzene	0.602	0.490	0.000	0.160	4.084	1.1391	−41.38	[43]
1,2-Dimethylbenzene	0.663	0.560	0.000	0.160	3.939	0.9982	−39.90	[27]
1,3-Dimethylbenzene	0.623	0.520	0.000	0.160	3.839	0.9982	−39.31	[43]
1,4-Dimethylbenzene	0.613	0.520	0.000	0.160	3.839	0.9982	−38.88	[27]
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3240	−62.65	[43]
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.7341	−34.98	[43]
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	−39.24	[43]
Bromobenzene	0.882	0.730	0.000	0.090	4.041	0.8914	−41.55	[43]
Iodobenzene	1.188	0.820	0.000	0.120	4.502	0.9746	−46.17	[43]
Nitrobenzene	0.871	1.110	0.000	0.280	4.557	0.8906	−53.89	[43]
Dichloromethane	0.387	0.570	0.100	0.050	2.019	0.4943	−27.62	[27]
Chloroform	0.425	0.490	0.150	0.020	2.480	0.6167	−32.19	[27]
1,2-Dichloroethane	0.416	0.640	0.100	0.110	2.573	0.6352	−32.47	[27]
trans-1,2-Dichloroethylene	0.425	0.410	0.090	0.050	2.278	0.5922	−29.00	[72]
Trichloroethylene	0.524	0.370	0.080	0.030	2.997	0.7146	−33.78	[72]
Tetrachloroethylene	0.639	0.440	0.000	0.000	3.584	0.8370	−36.51	[72]
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	−15.70	[76]
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237	−38.64	[55]
Sulfur dioxide	0.370	0.660	0.280	0.100	0.778	0.3465	−31.38	[77]
1-Bromoadamantane	1.070	0.900	0.000	0.200	6.130	1.3668	−52.30	[41]
1-Adamantanol	0.940	0.900	0.310	0.660	5.634	1.2505	−61.10	[41]

Each of the equation coefficients in the Abraham model encodes chemical information. For example the large *a*-coefficient in Eq. (8) indicates that dimethyl sulfoxide exhibits strong hydrogen-bonding basicity character, which is consistent with the molecule's molecular structure, $CH_3S(=O)CH_3$. The two lone electron pairs on the oxygen atom serve as acceptor sites for hydrogen-bond formation. The small, nonzero *b*-coefficient suggests a very weak hydrogen-bond acidity character. While dimethyl sulfoxide is not normally considered to possess any acidic hydrogen(s), several published studies have mentioned the possibility that one of the C–H hydrogens may engage in hydrogen bonding. Fujimoto et al. [92] rationalized the proton NMR spectra of solutions of dimethyl sulfoxide, 2-propanol and/or acetone with tetrasulfonated derivatives of calix[4]resorcarene dissolved in D_2O in terms of well-defined complexes resulting from CH–π interactions between the electron rich benzene rings on the calix[4]resorcarene derivatives and the polarized C–H bonds on the three guest molecules. The authors presented a very compelling argument for why CH–π interactions should be regarded as C–H···π hydrogen bonding. Leggett [93] had earlier estimated acidity parameters for solvents like dimethyl sulfoxide, propylene carbonate, *N*,*N*-dimethylformamide and butyrolactone that were believed to not possess hydrogen donor ability. At this time we do not place too much significance on the nonzero *b*-coefficient in Eq. (8) as it possible to still obtain a very good correlation:

$$\begin{aligned}\Delta H_{\text{Solv,DMSO}}\,(\text{kJ/mol}) &= -2.767(0.778) + 2.477(0.911)E - 22.053(1.062)S \\ &\quad - 50.701(1.724)A - 6.563(0.216)L \\ &\quad (\text{with } N = 150,\ \text{S.D.} = 3.11,\ R^2 = 0.969, \\ &\quad R^2_{\text{adj}} = 0.967,\ F = 539.1) \end{aligned} \qquad (10)$$

by setting the *b*-coefficient equal to zero. The standard deviation increased slightly from S.D. = 2.80 (Eq. (8)) to S.D. = 3.11 (Eq. (10)). Given the likely experimental uncertainty in the measured enthalpy of solvation data there is virtually no difference in the two correlations.

In order to assess the predictive ability of Eq. (8) we divided the 150 data points into a training set and a test set by allowing the SPSS software to randomly select half of the experimental data 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

$$\begin{aligned}
&\Delta H_{\text{Solv,DMSO}}\ (\text{kJ/mol})\\
&\quad = -4.505(0.928) + 1.003(1.406)E - 21.371(1.565)S\\
&\qquad - 47.478(2.190)A - 1.793(1.492)B - 5.816(0.272)L\\
&\quad (\text{with } N = 75,\ \text{S.D.} = 2.49,\ R^2 = 0.969,\\
&\quad R^2_{\text{adj}} = 0.967,\ F = 434.3) \qquad (11)
\end{aligned}$$

There is very little difference in the equation coefficients for the full dataset and 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 $\Delta H_{\text{Solv,DMSO}}$ values for the 75 compounds in the test set. For the predicted and experimental values, we find that S.D. = 3.57, AAE (average absolute error) = 2.288, and AE (average error) = −0.797. There is therefore very little bias in the predictions using Eq. (11) with AE equal to −0.797 kJ/mol.

In Table 2 are collected values of the enthalpies of solvation of 107 gaseous solutes in propylene carbonate. Regression analyses of the experimental $\Delta H_{\text{Solv,PC}}$ data in accordance with the Abraham model yielded:

$$\begin{aligned}
\Delta H_{\text{Solv,PC}} &= -4.377(0.791) + 0.478(1.510)E\\
&\quad - 13.370(1.526)S - 17.898(2.185)A\\
&\quad - 12.596(1.362)B - 6.685(0.299)L\\
&\quad (\text{with } N = 107,\ \text{S.D.} = 2.61,\ R^2 = 0.967,\\
&\quad R^2_{\text{adj}} = 0.965,\ F = 584.5) \qquad (12)
\end{aligned}$$

$$\begin{aligned}
\Delta H_{\text{Solv,PC}} &= 1.409(0.987) - 7.886(1.336)E - 18.776(1.535)S\\
&\quad - 20.632(2.205)A - 11.636(1.413)B\\
&\quad - 24.199(1.056)V\\
&\quad (\text{with } N = 107,\ \text{S.D.} = 2.55,\ R^2 = 0.964,\\
&\quad R^2_{\text{adj}} = 0.962,\ F = 564.9) \qquad (13)
\end{aligned}$$

Both Eqs. (12) and (13) are statistically very good with standard deviations of 2.61 and 2.55 kJ/mol for a data set that covers a range of 103.13 kJ/mol. Fig. 2 compares the calculated values of $\Delta H_{\text{Solv,PC}}$ based on Eq. (12) against the observed values. To our knowledge there has been no previous attempt to correlate $\Delta H_{\text{Solv,PC}}$ data.

We assessed the predictive ability of Eq. (12) by dividing the 107 data points into a training set and a test set as before. Analysis of the experimental data in the training set gave

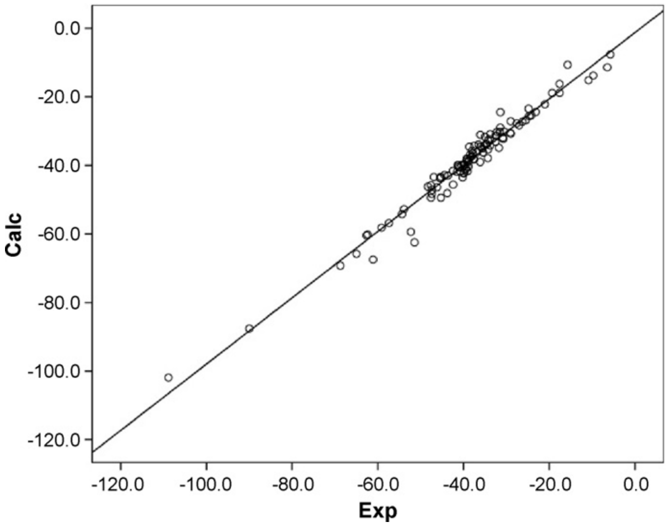

Fig. 2. A plot of the calculated values of $\Delta H_{\text{Solv,PC}}$ on Eq. (12) against the observed values.

$$\begin{aligned}
&\Delta H_{\text{Solv,PC}}\ (\text{kJ/mol})\\
&\quad = -1.618(0.924) + 2.630(1.953)E - 17.421(1.873)S\\
&\quad - 21.095(2.464)A - 10.426(1.606)B - 7.420(0.373)L \qquad (14)
\end{aligned}$$

with $N = 54$, S.D. = 2.03, $R^2 = 0.985$, $R^2_{\text{adj}} = 0.983$ and $F = 629.8$. There is very little difference in the equation coefficients for the full dataset and training dataset correlations. The training set equation was then used to predict $\Delta H_{\text{Solv,PC}}$ values for the 53 compounds in the test set. For the predicted and experimental values, we find that S.D. = 3.50 kJ/mol, AAE (average absolute error) = 3.46, and AE (average error) = 0.793. There is therefore very little bias in the predictions using Eq. (14) with AE equal to 0.793 kJ/mol. An uncertainty/error of ±2 kJ/mol 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 298.15–313.15 K. This level of error will be sufficient for most practical chemical and engineering applications.

The correlations presented in this study further document the applicability of the Abraham solvation parameter model to different solute transfer properties. Past studies have shown that the basic model describes a wide range of equilibrium properties that are governed by the Gibbs energy for solute transfer between two condensed phases or between a gas and condensed phase. In the present study we find that the model also provides an accurate mathematical description of the enthalpic contributions to the Gibbs energy, and by inference, we assume that the model describes the entropic contributions as well.

References

[1] D.M. Stovall, W.E. Acree Jr., M.H. Abraham, Fluid Phase Equilib. 232 (2005) 113.

[2] M.H. Abraham, W.E. Acree Jr., Int. J. Pharm. 294 (2005) 121.
[3] M.H. Abraham, A.M. Zissimos, W.E. Acree Jr., New J. Chem. 27 (2003) 1041.
[4] M.H. Abraham, A.M. Zissimos, J.G. Huddleston, H.D. Willauer, R.D. Rogers, W.E. Acree Jr., Ind. Eng. Chem. Res. 42 (2003) 413.
[5] M.H. Abraham, W.E. Acree Jr., New J. Chem. 28 (2004) 1538.
[6] M.H. Abraham, W.E. Acree Jr., Can. J. Chem. Eng. 83 (2005) 362.
[7] M.H. Abraham, Chem. Soc. Rev. 22 (1993) 73.
[8] M.H. Abraham, A. Ibrahim, A.M. Zissimos, J. Chromatogr. A 1037 (2004) 29.
[9] M.H. Abraham, H.S. Chadha, G.S. Whitting, R.C. Mitchell, J. Pharm. Sci. 83 (1994) 1085.
[10] M.H. Abraham, J. Le, J. Pharm. Sci. 88 (1999) 868.
[11] C. Mintz, M. Clark, W.E. Acree Jr., M.H. Abraham, J. Chem. Inf. Model. 47 (2007) 115.
[12] C. Mintz, M. Clark, K. Burton, W.E. Acree Jr., M.H. Abraham, QSAR Comb. Sci., in press, doi:10.1002/qsar.200630152.
[13] C. Mintz, M. Clark, K. Burton, W.E. Acree Jr., M.H. Abraham, J. Solut. Chem., in press.
[14] H. Ahmed, C.F. Poole, J. Sep. Sci. 29 (2006) 2158.
[15] J. Qian, C.F. Poole, J. Chromatogr. A 1143 (2007) 276.
[16] H. Ahmed, C.F. Poole, J. Chromatogr. A 1104 (2006) 82.
[17] W.K. Stephenson, R. Fuchs, Can. J. Chem. 63 (1985) 336.
[18] W.K. Stephenson, R. Fuchs, Can. J. Chem. 63 (1985) 342.
[19] C.V. Krishnan, H.L. Friedman, J. Phys. Chem. 75 (1971) 3598.
[20] T. Kimura, T. Tsuda, S. Takagi, Thermochim. Acta 267 (1995) 333.
[21] T. Kimura, K. Suzuki, S. Takagi, Fluid Phase Equilib. 136 (1997) 269.
[22] R. Francesconi, F. Comelli, A. Bigi, K. Rubini, Thermochim. Acta 447 (2006) 154.
[23] X. Hu, Y. Zhang, Z. Huang, Wuli Huaxue Xuebao 1 (1985) 130.
[24] F. Comelli, R. Francesconi, A. Bigi, K. Rubini, J. Chem. Eng. Data 51 (2006) 665.
[25] F. Comelli, S. Ottani, R. Francesconi, C. Castellari, J. Chem. Eng. Data 48 (2003) 995.
[26] R. Francesconi, A. Bigi, K. Rubini, F. Comelli, J. Chem. Eng. Data 50 (2005) 1932.
[27] M. Topphoff, D. Gruber, J. Gmehling, J. Chem. Eng. Data 44 (1999) 1355.
[28] J. Catalan, J. Gomez, A. Couto, J. Laynez, J. Am. Chem. Soc. 112 (1990) 1678.
[29] F.S. Costa, M.E. Eusebio, J.S. Redinha, M.L.P. Leitao, J. Chem. Thermodyn. 32 (2000) 311.
[30] A. Nissema, T. Kaivamo, M. Karvo, J. Chem. Thermodyn. 15 (1983) 1083.
[31] R. Philippe, Int. DATA Ser. Sel. Data Mix. Ser. A (1975) 122.
[32] R. Philippe, Int. DATA Ser. Sel. Data Mix. Ser. A (1975) 126.
[33] E.M. Arnett, D.R. McKelvey, J. Am. Chem. Soc. 88 (1966) 2598.
[34] M.H. Abraham, A. Nasehzadeh, J. Chem. Thermodyn. 13 (1981) 549.
[35] R.L. Benoit, M. Frechette, Thermochim. Acta 126 (1988) 155.
[36] J.H. Hallman, W.K. Stephenson, R. Fuchs, Can. J. Chem. 61 (1983) 2044.
[37] T. Matsui, L.G. Hepler, D.V. Fenby, J. Phys. Chem. 77 (1973) 2397.
[38] M. Jóźwiak, Thermochim. Acta 417 (2004) 31.
[39] M.D. Borisover, A.A. Stolov, F.D. Baitalov, A.I. Morozov, B.N. Solomonov, Thermochim. Acta 285 (1996) 199.
[40] F.S. Costa, M.E. Eusébio, J.S. Redinha, M.L.P. Leitão, J. Chem. Thermodyn. 31 (1999) 895.
[41] N. Nunes, L. Moreira, R.E. Leitão, F. Martins, J. Chem. Thermodyn., in press, doi:10.1016/j.jct.2006.12.002.
[42] G.R. Bebahani, D. Dunnion, P. Falvey, K. Hickey, M. Meade, Y. McCarthy, M.C.R. Symons, W.E. Waghorne, J. Solut. Chem. 29 (2000) 521.
[43] C.V. Krishnan, H.L. Friedman, J. Phys. Chem. 73 (1969) 1572.
[44] G. Pathak, A.D. Tripathi, S. Pradhan, Thermochim. Acta 197 (1992) 329.
[45] D. Figeys, M. Koschmidder, R.L. Benoit, Can. J. Chem. 70 (1992) 1586.
[46] N.G. Manin, S.Y. Belichenko, V.P. Korolev, Russ. J. Gen. Chem. 73 (2003) 9.
[47] R.L. Benoit, M.J. Mackinnon, L. Bergeron, Can. J. Chem. 59 (1981) 1501.
[48] T. Kimura, S. Takagi, Thermochim. Acta 253 (1995) 59.
[49] T. Kimura, S. Takagi, Netsu Sokutei 23 (1996) 53.
[50] K. Ohtsu, K. Ozutsumi, J. Incl. Phenom. Macrocycl. Chem. 45 (2003) 217.
[51] A.A.C.C. Pais, A. Sousa, M.E. Eusebio, J.S. Redinha, Phys. Chem. Chem. Phys. 3 (2001) 4001.
[52] B.G. Cox, J. Chem. Soc., Perkin Trans. 2 (1973) 607.
[53] D.V. Batov, O.A. Antonova, V.P. Korolev, Russ. J. Gen. Chem. 71 (2001) 689.
[54] R.L. Benoit, M. Frechette, D. Lefebvre, Can. J. Chem. 66 (1988) 1159.
[55] G.A. Krestov, V.P. Korolyov, D.V. Batov, Thermochim. Acta 169 (1990) 69.
[56] B.N. Solomonov, F.T. Khafizov, V.V. Gorbachuk, Zhur. Obsch. Khim. 60 (1990) 1446.
[57] W.K. Stephenson, R. Fuchs, Can. J. Chem. 63 (1985) 2529.
[58] W.K. Stephenson, R. Fuchs, Can. J. Chem. 63 (1985) 2535.
[59] R. Philippe, Int. DATA Ser. Sel. Data Mix. Ser. A (1975) 124.
[60] V.I. Smirnov, E.V. Kastorina, G.A. Kiestov, A.Ya. Fridman, Zhur. Fiz. Khim. 67 (1993) 1123.
[61] M. Lahti, A. Kankaanpera, H. Sapyska, J. Chem. Soc., Perkin Trans. 2 (1990) 1081.
[62] M.H. Abraham, J. Am. Chem. Soc. 104 (1982) 2085.
[63] F. Comelli, R. Francesconi, S. Ottani, J. Chem. Eng. Data 43 (1998) 333.
[64] F. Comelli, R. Francesconi, J. Chem. Eng. Data 40 (1995) 805.
[65] R. Francesconi, F. Comelli, J. Chem. Eng. Data 40 (1995) 811.
[66] F. Comelli, R. Francesconi, C. Castellari, J. Chem. Eng. Data 44 (1999) 144.
[67] C. Castellari, F. Comelli, R. Francesconi, Thermochim. Acta 413 (2004) 249.
[68] S. Ottani, F. Comelli, C. Castellari, J. Chem. Eng. Data 46 (2001) 125.
[69] F. Comelli, R. Francesconi, J. Chem. Eng. Data 50 (2005) 191.
[70] R. Francesconi, F. Comelli, J. Chem. Eng. Data 40 (1995) 31.
[71] K. Ohtsu, T. Kawashima, K. Ozutsumi, J. Chem. Soc., Faraday Trans. 91 (1995) 4375.
[72] R. Francesconi, F. Comelli, Thermochim. Acta 260 (1995) 95.
[73] A.F.D. de Namor, J.C.Y. Ng, M.A.L. Tanco, M. Salomon, J. Phys. Chem. 100 (1996) 14485.
[74] R. Francesconi, F. Comelli, J. Chem. Eng. Data 41 (1996) 1397.
[75] F. Comelli, R. Francesconi, C. Castellari, Thermochim. Acta 354 (2000) 89.
[76] F. Blanchard, B. Carre, F. Bonhomme, P. Biensan, D. Lemordant, Can. J. Chem. 81 (2003) 385.
[77] R.L. Benoit, E. Milanova, Can. J. Chem. 57 (1979) 1319.
[78] R. Fuchs, W.K. Stephenson, Can. J. Chem. 63 (1985) 349.
[79] T. Kimura, T. Matsushita, T. Kamiyama, J. Solut. Chem. 33 (2004) 875.
[80] T. Kimura, T. Matsushita, T. Kamiyama, Thermochim. Acta 416 (2004) 129.
[81] A. Gennaro, A.A. Isse, E. Vianello, J. Electroanal. Chem. Interfacial Electrochem. 289 (1990) 203.
[82] Y. Takeda, T. Watanabe, H. Yamada, S. Katsuta, J. Mol. Liq. 108 (2003) 151.
[83] M. Jozwiak, Thermochim. Acta 417 (2004) 31.
[84] J.S. Chickos, W.E. Acree Jr., J. Phys. Chem. Ref. Data 32 (2003) 519.
[85] J.S. Chickos, W.E. Acree Jr., J. Phys. Chem. Ref. Data 31 (2002) 537.
[86] PharmaAlgorithms, ADME Boxes, Version 3.0, PharmaAlgorithms Inc., 591 Indian Road, Toronto, Ont. M6P 2C4, Canada, 2006.
[87] J.A. Platts, D. Butina, M.H. Abraham, A. Hersey, J. Chem. Inf. Comp. Sci. 39 (1999) 835.
[88] J. Jover, R. Bosque, J. Sales, J. Chem. Inf. Comp. Sci. 44 (2004) 1098.
[89] J.S. Arey, W.H. Green Jr., P.M. Gschwend, J. Phys. Chem. B 109 (2005) 7564.
[90] F. Metelet, M. Rogalski, J. Chromatogr. A 923 (2001) 153.
[91] M.H. Abraham, J.C. McGowan, Chromatographia 23 (1987) 245.
[92] T. Fujimoto, R. Yanagihara, K. Kobayashi, Y. Aoyama, Bull. Chem. Soc. Jpn. 68 (1995) 2113.
[93] D.C. Leggett, J. Solut. Chem. 23 (1994) 697.