J. Braz. Chem. Soc., Vol. 19, No. 3, S1-S9, 2008.
Printed in Brazil - ©2008 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

Solubility Prediction of Solutes in Non-Aqueous Binary Solvent Mixtures

Abolghasem Jouyban,*[a] Maryam Khoubnasabjafari,[b] Somaieh Soltani,[c] Shahla Soltanpour,[d] Elnaz Tamizi[e] and William E. Acree Jr.[f]

[a]Faculty of Pharmacy and Drug Applied Research Center, Tabriz University of Medical Sciences, 51664, Iran

[b]Kimia Research Institute, P.O. Box 51665-171, Iran

[c]Research Center for Pharmaceutical Nanotechnology, Tabriz University of Medical Sciences, 51664, Iran

[d]Biotechnology Research Centre, Tabriz University of Medical Sciences, 51664, Iran

[e]Student Research Center, Tabriz University of Medical Sciences, 51664, Iran

[f]Department of Chemistry, University of North Texas, Denton, TX 76203-5070, USA

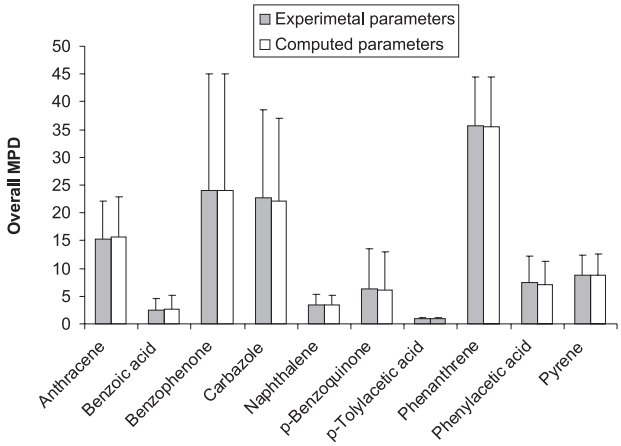

Figure S1. The overall *MPD* (± SD) for numerical method I for various solutes

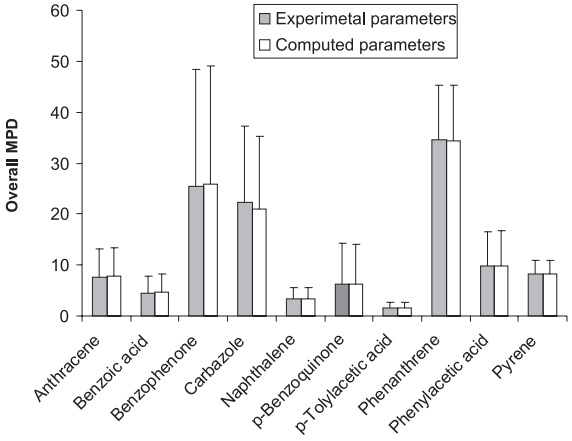

Figure S2. The overall *MPD* (± SD) for numerical method II for various solutes

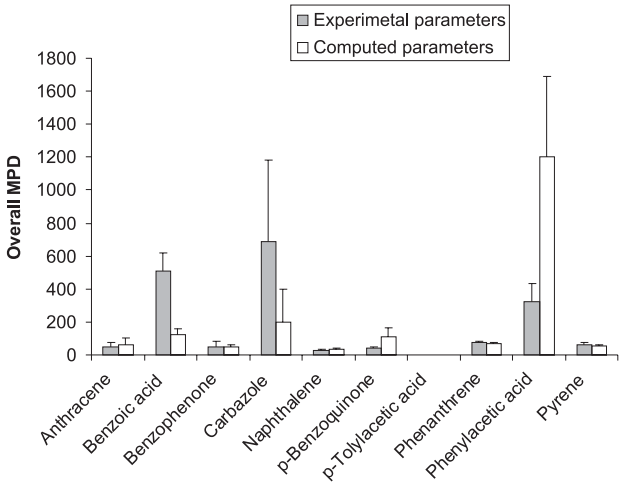

Figure S3. The overall *MPD* (± SD) for numerical method III for various solutes

*e-mail: ajouyban@hotmail.com

Table S1. Details of solutes and solvents names, the references of experimental data sets, logarithms of solubility in mono-solvents (lnX_1 and lnX_2) and temperature (T)

No.	Solute	Solvent 1	Solvent 2	N	Reference	lnX_1	lnX_2	T (°C)
1	Anthracene	Toluene	2-Propanol	11	11	-5.10	-8.57	20
2	Anthracene	Toluene	2-Propanol	11	11	-4.92	-7.90	25
3	Anthracene	Toluene	2-Propanol	11	11	-4.77	-7.76	30
4	Anthracene	Toluene	2-Propanol	11	11	-4.55	-7.46	35
5	Anthracene	Toluene	2-Propanol	11	11	-4.49	-7.21	40
6	Anthracene	Toluene	2-Propanol	11	11	-4.25	-7.22	45
7	Anthracene	Toluene	2-Propanol	11	11	-4.14	-6.82	50
8	Anthracene	Toluene	Heptane	10	11	-5.05	-6.72	20
9	Anthracene	Toluene	Heptane	10	11	-4.94	-6.61	25
10	Anthracene	Toluene	Heptane	10	11	-4.77	-6.29	30
11	Anthracene	Toluene	Heptane	10	11	-4.62	-6.34	35
12	Anthracene	Toluene	Heptane	10	11	-4.51	-6.05	40
13	Anthracene	Toluene	Heptane	10	11	-4.25	-5.72	45
14	Anthracene	Toluene	Heptane	10	11	-4.23	-5.68	50
15	Benzoic acid	Carbon tetrachloride	Cyclohexane	7	12	-3.01	-4.47	25
16	Benzoic acid	Carbon tetrachloride	Heptane	10	12	-3.01	-4.47	25
17	Benzoic acid	Carbon tetrachloride	Heptane	6	12	-2.82	-4.22	30
18	Benzoic acid	Carbon tetrachloride	Hexane	7	12	-3.01	-4.61	25
19	Benzoic acid	Carbon tetrachloride	Hexane	7	12	-2.82	-4.37	30
20	Benzoic acid	Cyclohexane	Heptane	7	12	-4.47	-4.47	25
21	Benzoic acid	Cyclohexane	Hexane	7	12	-4.47	-4.61	25
22	Benzoic acid	Cyclohexane	Hexane	7	12	-4.23	-4.37	30
23	Benzophenone	Carbon tetrachloride	Decane	11	13	-0.60	-3.03	25
24	Benzophenone	Carbon tetrachloride	Dodecane	11	13	-0.60	-3.54	25
25	Benzophenone	Carbon tetrachloride	Heptane	11	13	-0.60	-3.16	25
26	Benzophenone	Carbon tetrachloride	Hexane	9	13	-0.60	-3.75	25
27	Benzophenone	Carbon tetrachloride	Nonane	11	13	-0.60	-2.81	25
28	Benzophenone	Carbon tetrachloride	Octane	11	13	-0.60	-2.66	25
30	Carbazole	Cyclohexane	2,2,4-Trimethylpentane	11	14	-8.61	-8.98	25
31	Carbazole	Cyclohexane	Heptane	9	14	-8.61	-8.66	25
32	Carbazole	Cyclohexane	Hexane	9	14	-8.61	-8.88	25
29	Carbazole	Dibutylether	2,2,4-Trimethylpentane	9	15	-5.30	-8.98	25
33	Carbazole	Dibutylether	Cyclohexane	11	16	-5.30	-8.61	25
34	Carbazole	Dibutylether	Heptane	11	16	-5.30	-8.66	25
35	Carbazole	Dibutylether	Hexadecane	11	17	-5.30	-7.79	25
36	Carbazole	Dibutylether	Hexane	11	16	-5.30	-8.88	25
37	Carbazole	Dibutylether	Methylcyclohexane	11	15	-5.30	-8.54	25
38	Carbazole	Dibutylether	Methylcyclohexane	11	16	-5.30	-8.54	25
39	Carbazole	Dibutylether	n-Heptane	11	15	-5.30	-8.66	25
40	Carbazole	Dibutylether	n-Hexane	11	15	-5.30	-8.88	25
41	Carbazole	Dibutylether	n-Octane	11	15	-5.30	-8.53	25
42	Carbazole	Dibutylether	Octane	11	16	-5.30	-8.53	25
43	Carbazole	Methylcyclohexane	Cyclohexane	9	14	-8.54	-8.61	25
44	Carbazole	Octane	Cyclohexane	9	14	-8.53	-8.61	25
45	Naphthalene	Benzene	Carbon tetrachloride	6	18	-1.22	-1.35	25

Table S1. continuation

No.	Solute	Solvent 1	Solvent 2	N	Reference	lnX_1	lnX_2	T (°C)
46	Naphthalene	Benzene	Cyclohexane	8	18	-1.22	-1.91	25
47	Naphthalene	Benzene	Hexadecane	6	18	-1.22	-1.59	25
48	Naphthalene	Benzene	Hexane	8	18	-1.22	-2.15	25
49	Naphthalene	Benzene	Toluene	7	18	-1.22	-1.23	25
50	Naphthalene	Carbon tetrachloride	Cyclohexane	6	19	-1.35	-1.91	25
51	Naphthalene	Carbon tetrachloride	Hexadecane	6	19	-1.35	-1.59	25
52	Naphthalene	Carbon tetrachloride	Hexane	8	19	-1.35	-2.15	25
53	Naphthalene	Cyclohexane	Hexane	6	19	-1.91	-2.15	25
54	Naphthalene	Hexadecane	Cyclohexane	7	19	-1.59	-1.91	25
55	Naphthalene	Hexadecane	Hexane	6	19	-1.59	-2.15	25
56	Naphthalene	Toluene	Carbon tetrachloride	6	20	-1.23	-1.35	25
57	Naphthalene	Toluene	Cyclohexane	6	20	-1.23	-1.91	25
58	Naphthalene	Toluene	Hexadecane	6	20	-1.23	-1.59	25
59	Naphthalene	Toluene	Hexane	6	20	-1.23	-2.15	25
60	p-Benzoquinone	2,2,4-Trimethylpentane	Cyclohexane	7	21	-5.01	-5.03	25
61	p-Benzoquinone	Carbon tetrachloride	Heptane	8	21	-3.37	-5.01	25
62	p-Benzoquinone	Carbon tetrachloride	Octane	7	21	-3.37	-4.89	25
63	p-Benzoquinone	Dodecane	Heptane	7	21	-4.74	-5.01	25
64	p-Benzoquinone	Heptane	Cyclohexane	7	21	-5.01	-5.03	25
65	p-Tolylacetic acid	Cyclohexane	2,2,4-Trimethylpentane	7	22	-4.32	-4.83	25
66	p-Tolylacetic acid	Cyclohexane	Heptane	7	22	-4.30	-4.78	25
67	p-Tolylacetic acid	Cyclohexane	Hexane	8	22	-4.32	-4.85	25
68	p-Tolylacetic acid	Cyclohexane	Octane	7	22	-4.32	-4.75	25
69	Phenanthrene	Toluene	2,2,4-Trimethylpentane	7	23	-0.77	-3.96	20
70	Phenanthrene	Toluene	2,2,4-Trimethylpentane	7	23	-0.70	-3.32	30
71	Phenanthrene	Toluene	2,2,4-Trimethylpentane	7	23	-0.55	-2.44	40
72	Phenanthrene	Toluene	2,2,4-Trimethylpentane	7	23	-0.50	-1.98	50
73	Phenanthrene	Toluene	Heptane	11	23	-0.77	-4.17	20
74	Phenanthrene	Toluene	Heptane	11	23	-0.70	-3.70	30
75	Phenanthrene	Toluene	Heptane	11	23	-0.55	-3.32	40
76	Phenanthrene	Toluene	Heptane	11	23	-0.50	-2.96	50
77	Phenylacetic acid	Carbon tetrachloride	2,2,4-Trimethylpentane	11	24	-1.75	-4.40	25
78	Phenylacetic acid	Carbon tetrachloride	Cyclohexane	11	24	-1.75	-3.70	25
79	Phenylacetic acid	Carbon tetrachloride	Heptane	11	24	-1.75	-4.31	25
80	Phenylacetic acid	Carbon tetrachloride	Octane	11	24	-1.75	-4.24	25
81	Phenylacetic acid	Cyclohexane	2,2,4-Trimethylpentane	9	24	-3.70	-4.40	25
82	Phenylacetic acid	Cyclohexane	Heptane	8	24	-3.70	-4.31	25
83	Pyrene	Toluene	2,2,4-Trimethylpentane	12	20	-2.87	-4.72	20
84	Pyrene	Toluene	2,2,4-Trimethylpentane	12	20	-2.41	-4.47	30
85	Pyrene	Toluene	2,2,4-Trimethylpentane	12	20	-2.21	-4.37	40
86	Pyrene	Toluene	2,2,4-Trimethylpentane	12	20	-1.57	-3.94	50
87	Pyrene	Toluene	Heptane	11	20	-2.87	-4.47	20
88	Pyrene	Toluene	Heptane	11	20	-2.41	-4.17	30
89	Pyrene	Toluene	Heptane	11	20	-2.21	-3.63	40
90	Pyrene	Toluene	Heptane	11	20	-1.57	-3.01	50

Table S2. Coefficients in equations (1) and (2) for water-to-solvent and gas-to-solvent processes of the solvents used in this study[a]

No.	Water-to-solvent coefficients	c	e	s	a	b	v
1	2,2,4-Trimethylpentane	0.288	0.382	-1.668	-3.639	-5.000	4.461
2	2-Propanol	0.063	0.320	-1.024	0.445	-3.824	4.067
3	Benzene	0.142	0.464	-0.588	-3.099	-4.625	4.491
4	Carbone tetrachloride	0.260	0.573	-1.254	-3.558	-4.558	4.589
5	Cyclohexane	0.159	0.784	-1.678	-3.740	-4.929	4.577
6	Decane	0.160	0.585	-1.730	-3.440	-5.080	4.582
7	Dibutyl ether	0.203	0.369	-0.954	-1.488	-5.426	4.508
8	Dodecane	0.114	0.668	-1.640	-3.550	-5.010	4.459
9	Heptane	0.325	0.670	-2.061	-3.317	-4.733	4.543
10	Hexadecane	0.087	0.667	-1.620	-3.59	-4.870	4.433
11	Hexane	0.361	0.579	-1.723	-3.599	-4.764	4.344
12	Methylcyclohexane	0.246	0.782	-1.982	-3.517	-4.293	4.528
13	Nonane	0.240	0.619	-1.710	-3.530	-4.920	4.482
14	Octane	0.223	0.642	-1.647	-3.480	-5.067	4.526
15	Toluene	0.143	0.527	-0.720	-3.010	-4.824	4.545
No.	Gas-to-solvent coefficients	c	e	s	a	b	l
1	2,2,4-Trimethylpentane	0.275	–0.244	0.000	0.000	0.000	0.972
2	2-Propanol	-0.060	-0.335	0.702	4.017	1.040	0.893
3	Benzene	0.107	–0.313	1.053	0.457	0.169	1.020
4	Carbone tetrachloride	0.282	–0.303	0.460	0.000	0.000	1.047
5	Cyclohexane	0.163	-0.110	0.000	0.000	0.000	1.013
6	Decane	0.156	-0.140	0.000	0.000	0.000	0.989
7	Dibutyl ether	0.165	–0.421	0.760	2.102	–0.664	1.002
8	Dodecane	0.053	0.000	0.000	0.000	0.000	0.986
9	Heptane	0.275	–0.162	0.000	0.000	0.000	0.983
10	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000
11	Hexane	0.292	–0.169	0.000	0.000	0.000	0.979
12	Methylcyclohexane	0.318	–0.215	0.000	0.000	0.000	1.012
13	Nonane	0.200	-0.145	0.000	0.000	0.000	0.980
14	Octane	0.215	–0.049	0.000	0.000	0.000	0.967
15	Toluene	0.121	–0.222	0.938	0.467	0.099	1.012

[a] Data taken from a reference.[5]

Table S3. The experimental and computed Abraham parameters along with the input properties for solutes studied in this work and their references

Solute	E	S	*A*	*B*	*V*	*L*	log C_W	log C_G	Reference
	Experimental Abraham parameters								
Anthracene	2.290	1.34	0.000	0.280		7.568	-6.430	-9.460	2
Benzoic acid	0.730	0.90	0.590	0.400		4.395	-1.550	-6.690	27
Benzophenone	1.447	1.50	0.000	0.500		6.852	-3.120[28]	-[a]	25
Carbazole	1.787	2.01	0.180	0.080		7.982	-5.270[28]	-[a]	25
Naphthalene	1.340	0.92	0.000	0.200		5.161	-3.610[29]	-5.340	30
p-Benzoquinone	0.750	0.55	0.000	0.810		3.492	-0.880[31]	-[a]	25
p-Tolylacetic acid	0.730	0.97	0.600	0.640		5.480	-[a]	-[a]	25
Phenanthrene	2.055	1.29	0.000	0.290		7.632	-5.170	-7.970	2
Phenylacetic acid	0.730	1.01	0.590	0.610		4.933	-0.890[28]	-7.562[b]	25
Pyrene	2.808	1.71	0.000	0.280		8.833	-6.150	-9.650	5
	Computed Abraham parameters								
Anthracene	1.99	1.34	0.000	0.23	1.454	7.706			25
Benzoic acid	0.75	1.08	0.570	0.44	0.932	4.533			25
Benzophenone	1.37	1.59	0.000	0.51	1.481	7.308			25
Carbazole	1.94	1.43	0.310	0.39	1.315	7.869			25
Naphthalene	1.27	1.02	0.000	0.17	1.085	5.332			25
p-Benzoquinone	0.90	0.43	0.000	0.76	0.791	3.500			25
p-Tolylacetic acid	0.77	1.02	0.570	0.45	1.214	5.499			25
Phenanthrene	1.99	1.34	0.000	0.23	1.454	7.706			25
Phenylacetic acid	0.75	1.08	0.570	0.45	1.073	5.028			25
Pyrene	2.60	1.52	0.000	0.25	1.585	9.110			25

[a] The data was not available.

[b] $\log C_G$ of phenylacetic acid was calculated using the extrapolated vapor pressure data from a reference[32] as: $\log C_G = \frac{6.796\times10^{-2}\ (vapor\ \ pressure)}{298.15\times0.08206\times101325}$.

Table S4. The individual percentage deviations (*IPD*s) of solubilities of solutes[10] in some of the solvents predicted by equations (1) and (2) employing experimental and computed Abraham parameters

Solute[a]	Solvent[a]	*T* (°C)	Experimental parameters		Computed parameters	
			Equation (1)	Equation (2)	Equation (1)	Equation (2)
Anthracene	1,4-Dioxane	25	20.5	20.0	64.4	36.1
Anthracene	1-Butanol	25	25.5	1.0	45.6	43.7
Anthracene	1-Octanol	25	17.0	23.9	35.7	8.8
Anthracene	1-Pentanol	25	34.4	21.9	47.0	13.5
Anthracene	2,2,4-Trimethylpentane	25	40.3	36.3	18.5	2.6
Anthracene	2-Butanol	25	21.2	24.0	55.6	22.8
Anthracene	2-Methyl-1-propanol	25	37.7	11.7	64.8	34.1
Anthracene	2-Propanol	25	28.5	5.4	60.0	40.4
Anthracene	Acetonitrile	25	14.6	6.3	80.0	70.1
Anthracene	Benzene	25	97.7	52.7	143.6	155.2
Anthracene	Carbon tetrachloride	25	49.3	3.3	69.7	65.7
Anthracene	Cyclohexane	25	149.6	7.7	156.1	37.3
Anthracene	Dibutyl ether	25	11.5	32.4	61.2	33.8
Anthracene	Heptane	25	16.7	28.2	9.6	9.7
Anthracene	Hexane	25	12.0	26.2	2.0	13.2
Anthracene	Methanol	25	3.2	1.8	24.0	27.9
Anthracene	Methyl tert-buthyl ether	25	22.6	24.6	82.0	44.6
Anthracene	Methylcyclohexane	25	66.8	17.8	59.4	31.4
Anthracene	Octane	25	46.8	18.7	68.8	14.3
Anthracene	Toluene	25	132.9	78.7	181.0	182.0
Benzil	1-Butanol	25	5.3	15.8	94.8	1599.5
Benzil	1-Octanol	25	60.1	29.0	91.8	1540.8
Benzil	1-Pentanol	25	10.9	95.6	95.1	1421.3
Benzil	1-Propanol	25	5.7	25.1	94.9	1146.8
Benzil	2,2,4-Trimethylpentane	25	38.2	29.4	99.0	375.6
Benzil	2-Butanol	25	46.5	32.3	91.0	2172.1
Benzil	2-Propanol	25	25.4	14.0	92.6	1882.9
Benzil	Carbon tetrachloride	25	38.6	51.6	97.8	337.6
Benzil	Cyclohexane	25	4.2	36.7	98.0	373.9
Benzil	Heptane	25	34.2	10.9	99.1	521.9
Benzil	Octane	25	25.6	14.2	97.7	498.8
Pyrene	1-Butanol	26	33.8	42.0	17.2	115.8
Pyrene	1-Octanol	26	39.8	1.9	0.0	45.3
Pyrene	1-Pentanol	26	34.0	43.1	18.1	16.8
Pyrene	1-Propanol	26	21.2	13.8	35.0	26.1
Pyrene	2,2,4-Trimethylpentane	26	75.4	23.1	40.1	59.7
Pyrene	2-Butanol	26	36.8	2.8	11.0	50.2
Pyrene	2-Methyl-1-propanol	26	26.4	21.0	29.4	77.3
Pyrene	2-Propanol	26	27.7	41.5	26.2	100.7
Pyrene	Benzene	26	64.4	210.3	124.4	300.3
Pyrene	Cyclohexane	26	59.5	38.1	215.3	173.6
Pyrene	Dibutyl ether	26	32.0	9.7	23.6	86.4
Pyrene	Heptane	26	66.0	5.7	16.1	88.8
Pyrene	Hexane	26	57.4	0.0	5.2	100.7
Pyrene	Methylcyclohexane	26	25.8	1.2	61.5	105.9
Pyrene	Octane	26	23.5	8.7	62.1	103.4
Thianthrene	2,2,4-Trimethylpentane	25	45.2	27.1	71.1	112.5
Thianthrene	Cyclohexane	25	53.1	22.9	29.4	121.9
Thianthrene	Heptane	25	12.3	3.1	56.2	176.4
Thianthrene	Hexane	25	17.7	12.6	58.4	149.3
Thianthrene	Methylcyclohexane	25	8.3	31.8	45.5	103.9

Table S4. continuation

Solute[a]	Solvent[a]	*T* (°C)	Experimental parameters		Computed parameters	
			Equation (1)	Equation (2)	Equation (1)	Equation (2)
Thianthrene	Octane	25	57.1	7.7	25.1	189.8
Trans-Stilbene	1-Propanol	25	23.4	10.8	33.9	57.4
Trans-Stilbene	2,2,4-Trimethylpentane	25	22.2	9.5	16.7	63.0
Trans-Stilbene	2-Butanol	25	53.2	28.5	79.9	32.5
Trans-Stilbene	Cyclohexane	25	32.2	14.5	22.7	67.7
Trans-Stilbene	Heptane	25	6.0	5.4	23.9	62.6
Trans-Stilbene	Hexane	25	17.7	8.7	22.0	63.7
Trans-Stilbene	Methylcyclohexane	25	21.4	4.3	8.8	62.5
Trans-Stilbene	Octane	25	27.2	11.9	27.5	65.9
Anthracene	1,4-Dioxane	25	20.5	20.0	64.4	36.1
		All	36.3[b]	24.4[c]	59.7[b]	262.8[c]
		25	34.6[d]	22.2[e]	64.5[d]	319.4[e]

[a] Details of the references of data were reported in an earlier work.[10]; [b] The difference was statistically significant (paired t-test, $p<0.0005$); [c] The difference was statistically significant (paired t-test, $p<0.0005$); [d] The difference was statistically significant (paired t-test, $p<0.0005$); [e] The difference was statistically significant (paired t-test, $p>0.001$).

Table S5. The mean percentage deviation (*MPD*) of various numerical analyses employing the experimental and computed Abraham parameters of the solutes and the overall (± SD) of *MPD*s

Numerical method No.[a]	I	II	III	IV	I	II	III	IV
	Experimental Abraham parameters				Computed Abraham parameters			
1	30.3	18.2	95.8	72.9	31.0	18.7	138.0	161.3
2	18.3	3.6	45.2	28.8	19.1	4.1	76.4	94.8
3	17.7	4.5	27.1	17.6	18.6	5.0	53.5	69.8
4	16.9	1.6	23.0	21.1	17.8	1.9	22.5	32.3
5	15.9	3.8	29.5	28.9	16.7	4.1	24.3	24.2
6	22.2	7.3	33.2	37.5	23.0	8.0	26.2	20.8
7	16.5	2.2	43.3	48.5	17.3	2.5	36.0	30.0
8	16.9	14.8	112.2	68.2	16.9	14.8	145.8	160.0
9	11.6	9.7	79.3	44.0	11.6	9.7	106.8	119.1
10	16.1	14.2	52.7	27.3	16.1	14.2	74.8	81.5
11	2.7	2.2	34.2	23.1	2.7	2.2	47.8	49.6
12	5.7	4.4	32.0	26.9	5.7	4.4	41.3	39.9
13	16.0	13.9	26.2	31.9	16.0	14.0	31.5	27.9
14	7.6	5.9	28.5	38.8	7.6	6.0	31.1	27.1
15	0.8	0.7	493.7	94.4	0.7	0.6	135.8	91.5
16	6.5	10.0	460.9	93.4	7.2	10.5	115.4	90.0
17	5.1	8.4	357.9	94.6	5.6	8.8	69.6	92.0
18	2.1	5.3	510.0	93.5	2.3	5.7	141.0	90.3
19	2.6	5.2	386.3	94.8	2.8	5.5	91.8	92.2
20	1.0	1.5	626.6	92.9	0.8	1.5	138.3	90.3
21	0.5	1.7	697.2	92.9	0.5	1.7	176.4	90.3
22	0.7	2.1	527.9	94.4	0.7	2.1	117.5	92.3
23	6.9	8.9	23.9	-	7.0	9.5	43.5	-
24	61.6	67.3	114.6	-	61.8	68.4	43.1	-
25	15.0	13.9	37.9	-	14.9	13.8	62.4	-
26	34.8	36.8	37.4	-	34.9	37.2	25.1	-
27	7.4	10.7	25.8	-	7.4	11.2	47.9	-
28	18.1	15.4	38.4	-	18.0	15.4	59.2	-
29	34.9	31.7	324.3	-	34.8	29.8	53.1	-
30	0.9	4.5	1291.2	-	0.9	4.4	370.3	-
31	0.9	0.8	1011.5	-	0.9	0.8	409.3	-
32	1.7	0.8	1355.5	-	1.9	0.8	461.7	-
33	41.4	39.4	596.9	-	41.1	38.0	118.1	-
34	28.2	29.8	231.9	-	27.7	27.9	50.6	-
35	16.7	14.3	528.2	-	15.6	11.9	65.3	-

Table S5. Cont.

Numerical method	I	II	III	IV	I	II	III	IV
No.[a]	Experimental Abraham parameters				Computed Abraham parameters			
36	35.5	34.5	348.6	-	34.4	32.9	61.1	-
37	36.2	37.2	282.8	-	32.2	35.8	87.7	-
38	35.6	36.6	268.2	-	31.0	35.0	87.3	-
39	28.2	29.8	231.9	-	27.7	27.9	50.6	-
40	35.5	34.5	349.0	-	34.3	32.8	61.2	-
41	32.2	28.3	581.9	-	32.3	26.4	83.7	-
42	32.2	28.3	581.9	-	32.3	26.4	83.7	-
43	2.2	0.6	1208.1	-	5.3	0.6	602.1	-
44	1.3	3.3	1811.2	-	1.1	3.3	547.9	-
45	2.4	3.5	23.1	16.3	2.6	3.7	21.3	30.7
46	4.7	3.5	26.5	31.5	4.3	3.1	28.6	22.7
47	1.9	4.1	26.8	12.8	2.2	4.6	29.5	26.8
48	5.4	4.2	36.7	27.6	5.0	3.8	38.0	18.2
49	1.1	1.3	11.2	3.6	1.1	1.4	4.7	48.6
50	1.9	0.7	32.4	39.1	2.0	0.5	39.3	11.2
51	6.0	8.4	30.3	17.5	6.0	8.5	36.9	18.4
52	2.0	1.1	42.0	33.2	2.0	1.4	47.7	5.6
53	1.1	0.3	37.6	41.7	1.1	0.3	46.5	15.1
54	6.4	6.2	28.3	25.7	6.4	6.2	37.4	11.0
55	4.7	2.6	36.7	25.6	4.7	2.7	44.7	7.5
56	2.1	3.4	18.7	12.3	2.1	3.6	17.9	34.2
57	5.1	3.3	22.3	27.5	4.7	3.0	25.0	23.5
58	2.1	3.6	23.1	9.9	2.3	4.0	26.4	29.2
59	5.2	5.1	32.7	24.7	4.8	4.7	34.7	18.2
60	0.2	1.1	45.5	-	.2	1.1	88.3	-
61	10.0	12.7	42.0	-	9.5	12.5	96.1	-
62	17.2	17.0	52.5	-	16.6	16.7	51.4	-
63	3.3	0.3	28.9	-	3.1	0.3	160.3	-
64	1.0	0.2	27.7	-	.9	0.2	167.5	-
65	1.1	0.7	-	-	1.1	0.7	-	-
66	1.1	0.5	-	-	1.0	0.5	-	-
67	0.9	2.6	-	-	1.0	2.6	-	-
68	0.5	2.3	-	-	0.5	2.3	-	-
69	36.0	33.4	70.1	40.3	35.9	33.3	54.8	35.2
70	31.2	28.3	77.3	49.9	31.1	28.1	65.8	39.0
71	26.5	23.3	84.5	66.9	26.4	23.1	76.7	59.8
72	20.3	16.7	86.1	70.8	20.2	16.4	79.1	64.4
73	42.2	43.0	61.7	55.2	42.1	42.9	52.4	53.0
74	45.1	45.8	71.3	56.0	44.9	45.7	59.6	50.4
75	43.3	44.1	77.1	58.2	43.1	43.9	67.4	53.1
76	40.5	41.4	80.3	61.9	40.3	41.2	71.8	54.0
77	11.4	16.5	274.9	98.3	10.4	16.8	994.3	97.9
78	6.4	6.6	158.9	99.0	6.9	6.5	620.2	98.8
79	6.1	9.3	263.2	98.4	6.2	9.5	901.2	97.9
80	14.7	19.3	323.8	98.3	13.4	19.5	1096.2	97.9
81	2.1	4.0	439.8	97.9	2.1	4.0	1823.2	97.4
82	3.7	3.0	458.7	97.8	3.6	3.0	1769.7	97.3
83	8.1	11.3	58.9	80.5	8.1	10.4	55.9	166.5
84	6.7	4.8	60.1	50.1	7.0	5.0	46.7	70.7
85	16.8	12.5	66.0	49.1	17.3	13.1	51.7	40.8
86	8.6	7.1	78.3	48.0	8.8	7.3	61.9	25.0
87	6.7	6.8	50.0	101.5	6.5	7.4	70.9	197.5
88	11.0	9.6	43.9	65.1	10.2	9.0	43.7	119.7
89	7.9	8.1	54.0	48.4	7.9	8.3	40.5	59.6
90	4.7	5.3	74.9	48.9	4.9	5.8	58.3	34.4
Overall:	13.7	12.7	228.7	53.5	13.6	12.5	168.9	62.7
SD	14.0	13.9	337.7	30.0	13.8	13.7	325.4	43.6

[a] Details of the data is the same as Table S1.

Table S6. The individual percentage deviations (*IPD*s) of solubilities of solutes in some of the solvents of this work predicted by equations (1) and (2) employing experimental and computed Abraham parameters

Solute	Solvent	*T* (°C)	Experimental parameters		Computed parameters	
			equation (1)	equation (2)	equation (1)	equation (2)
Anthracene	2-Propanol	20	180.1	105.3	248.7	204.8
Anthracene	2-Propanol	25	43.1	4.9	78.1	55.7
Anthracene	2-Propanol	30	24.3	8.9	54.7	35.2
Anthracene	2-Propanol	35	7.9	32.5	14.6	0.2
Anthracene	2-Propanol	40	28.5	47.6	10.9	22.2
Anthracene	2-Propanol	45	27.8	47.1	10.1	21.4
Anthracene	2-Propanol	50	51.5	64.5	39.7	47.2
Anthracene	Heptane	20	8.9	6.5	18.2	42.9
Anthracene	Heptane	25	2.9	16.7	5.4	27.3
Anthracene	Heptane	30	29.3	39.3	23.3	7.3
Anthracene	Heptane	35	25.8	36.3	19.5	2.7
Anthracene	Heptane	40	44.1	52.0	39.4	26.7
Anthracene	Heptane	45	59.8	65.5	56.4	47.3
Anthracene	Heptane	50	61.8	67.2	58.5	49.9
Anthracene	Toluene	20	181.9	115.5	240.1	239.9
Anthracene	Toluene	20	169.4	105.9	225.0	224.8
Anthracene	Toluene	25	136.4	80.7	185.2	185.0
Anthracene	Toluene	25	139.4	83.0	188.9	188.7
Anthracene	Toluene	30	102.3	54.7	144.1	144.0
Anthracene	Toluene	35	63.4	24.9	97.1	97.0
Anthracene	Toluene	35	74.8	33.6	110.9	110.8
Anthracene	Toluene	40	53.7	17.5	85.5	85.4
Anthracene	Toluene	40	57.1	20.0	89.5	89.4
Anthracene	Toluene	45	20.9	7.6	45.8	45.8
Anthracene	Toluene	50	8.1	17.3	30.5	30.4
Anthracene	Toluene	50	18.5	9.4	43.0	42.9
Benzoic acid	Carbon tetrachloride	25	336.2	95.2	100.8	92.1
Benzoic acid	Carbon tetrachloride	30	258.9	96.1	65.2	93.5
Benzoic acid	Cyclohexane	25	690.6	93.4	176.6	90.9
Benzoic acid	Cyclohexane	30	522.7	94.8	117.8	92.9
Benzoic acid	Heptane	25	569.9	92.1	101.2	89.3
Benzoic acid	Heptane	30	419.5	93.9	56.0	91.7
Benzoic acid	Hexane	25	708.0	92.1	177.1	89.2
Benzoic acid	Hexane	30	541.2	93.7	119.9	91.5
Benzophenone	Carbon tetrachloride	25	49.2	-	64.4	-
Benzophenone	Decane	25	28.7	-	25.9	-
Benzophenone	Dodecane	25	182.0	-	64.7	-
Benzophenone	Heptane	25	7.6	-	51.1	-
Benzophenone	Hexane	25	87.7	-	8.3	-
Benzophenone	Nonane	25	15.4	-	33.2	-
Benzophenone	Octane	25	15.7	-	32.3	-
Carbazole	2,2,4-Trimethylpentane	25	761.8	-	158.0	-
Carbazole	Cyclohexane	25	1967.8	-	661.6	-
Carbazole	Dibutyl ether	25	391.4	-	57.4	-
Carbazole	Heptane	25	333.7	-	193.8	-
Carbazole	Hexadecane	25	1017.3	-	280.2	-
Carbazole	Hexane	25	835.7	-	282.4	-
Carbazole	Methyl cyclohexane	25	557.4	-	470.5	-
Carbazole	Heptane	25	333.7	-	193.8	-
Carbazole	Hexane	25	835.7	-	282.4	-
Carbazole	Octane	25	1692.0	-	445.9	-

Table S6. continuation

Solute	Solvent	*T* (°C)	Experimental parameters		Computed parameters	
			equation (1)	equation (2)	equation (1)	equation (2)
Naphthalene	Benzene	25	16.5	8.7	9.4	43.0
Naphthalene	Carbon tetrachloride	25	33.6	29.8	37.1	8.7
Naphthalene	Cyclohexane	25	28.7	46.1	39.0	21.6
Naphthalene	Hexadecane	25	34.7	20.5	42.4	9.3
Naphthalene	Hexane	25	46.6	37.3	54.1	8.7
Naphthalene	Toluene	25	6.6	0.4	0.9	51.1
p-Benzoquinone	2,2,4-Trimethylpentane	25	54.8	-	44.4	-
p-Benzoquinone	Carbon tetrachloride	25	68.0	-	8.8	-
p-Benzoquinone	Cyclohexane	25	37.6	-	126.9	-
p-Benzoquinone	Dodecane	25	47.5	-	83.3	-
p-Benzoquinone	Heptane	25	16.7	-	215.2	-
p-Benzoquinone	Octane	25	45.7	-	89.6	-
Phenanthrene	2,2,4-Trimethylpentane	20	46.7	41.8	17.6	72.5
Phenanthrene	2,2,4-Trimethylpentane	30	71.9	25.2	56.5	9.0
Phenanthrene	2,2,4-Trimethylpentane	40	88.4	69.2	82.1	62.5
Phenanthrene	2,2,4-Trimethylpentane	50	92.7	80.4	88.6	76.2
Phenanthrene	Heptane	20	20.5	173.4	64.2	228.3
Phenanthrene	Heptane	30	24.9	70.5	2.4	104.7
Phenanthrene	Heptane	40	48.5	17.0	29.8	40.4
Phenanthrene	Heptane	50	64.3	18.9	51.3	2.6
Phenanthrene	Toluene	20	59.1	29.2	39.7	14.2
Phenanthrene	Toluene	30	62.1	34.5	44.2	20.7
Phenanthrene	Toluene	40	67.3	43.4	51.7	31.4
Phenanthrene	Toluene	50	68.7	45.9	53.9	34.5
Phenyl acetic acid	2,2,4-Trimethylpentane	25	561.6	97.1	2363.6	96.5
Phenyl acetic acid	Carbon tetrachloride	25	76.9	99.3	283.1	99.0
Phenyl acetic acid	Cyclohexane	25	339.2	98.6	1405.1	98.2
Phenyl acetic acid	Heptane	25	574.0	96.9	2107.4	96.2
Phenyl acetic acid	Octane	25	701.5	97.2	2677.3	96.6
Pyrene	2,2,4-Trimethylpentane	20	80.2	37.8	51.7	29.3
Pyrene	2,2,4-Trimethylpentane	30	84.5	51.4	62.3	0.9
Pyrene	2,2,4-Trimethylpentane	40	86.1	56.4	66.2	9.4
Pyrene	2,2,4-Trimethylpentane	50	90.9	71.5	77.9	40.7
Pyrene	Heptane	20	67.2	8.8	19.2	82.6
Pyrene	Heptane	30	75.7	32.5	40.2	35.2
Pyrene	Heptane	40	85.8	60.6	65.1	21.1
Pyrene	Heptane	50	92.5	79.0	81.4	57.9
Pyrene	Toluene	20	105.4	284.4	188.8	394.2
Pyrene	Toluene	30	30.2	143.6	83.0	213.2
Pyrene	Toluene	40	6.4	99.2	49.6	156.1
Pyrene	Toluene	50	43.8	5.2	21.0	35.2
		All	207.2[a]	59.1[b]	188.0[a]	73.6[b]
		25	343.6[c]	62.6[d]	331.1[c]	76.2[d]

[a] The difference was not statistically significant (paired t-test, p>0.05); [b] The difference was statistically significant (paired t-test, p<0.008); [c] The difference was not statistically significant (paired t-test, p>0.05); [d] The difference was not statistically significant (paired t-test, p>0.05).