Supporting information on

In silico prediction of linear free energy relationship descriptors of neutral and ionic compounds

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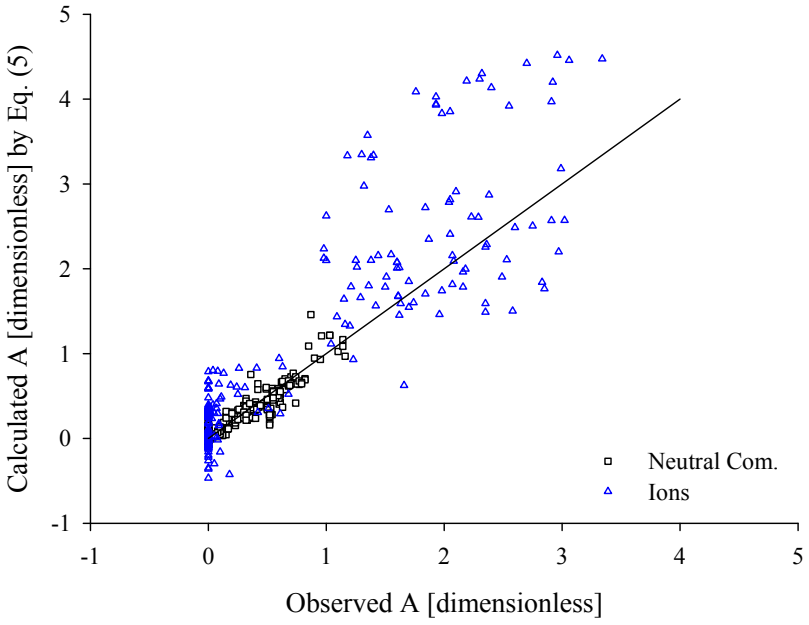
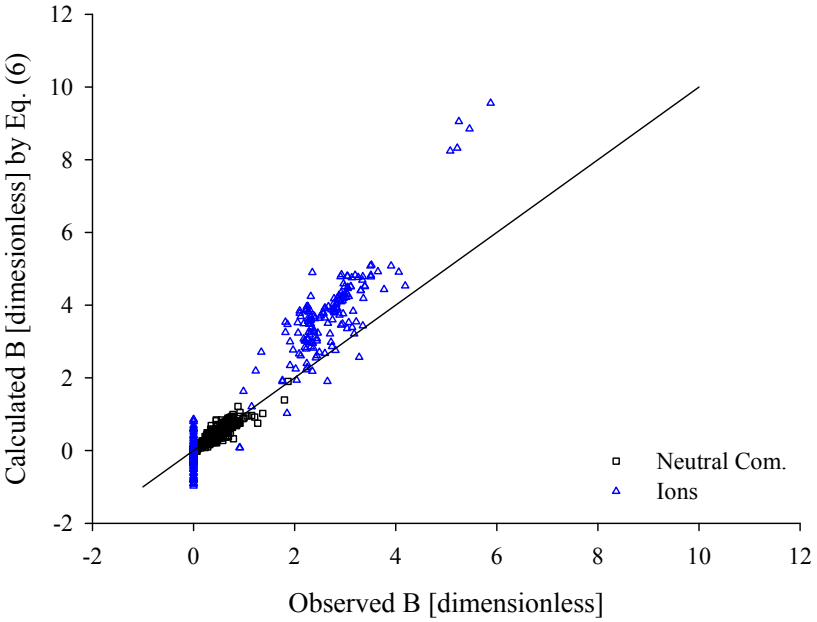
Fig. S1 Correlations of Abraham and calculated descriptors (A and B) according to Eqs. (5)-(6).

(A)



(B)



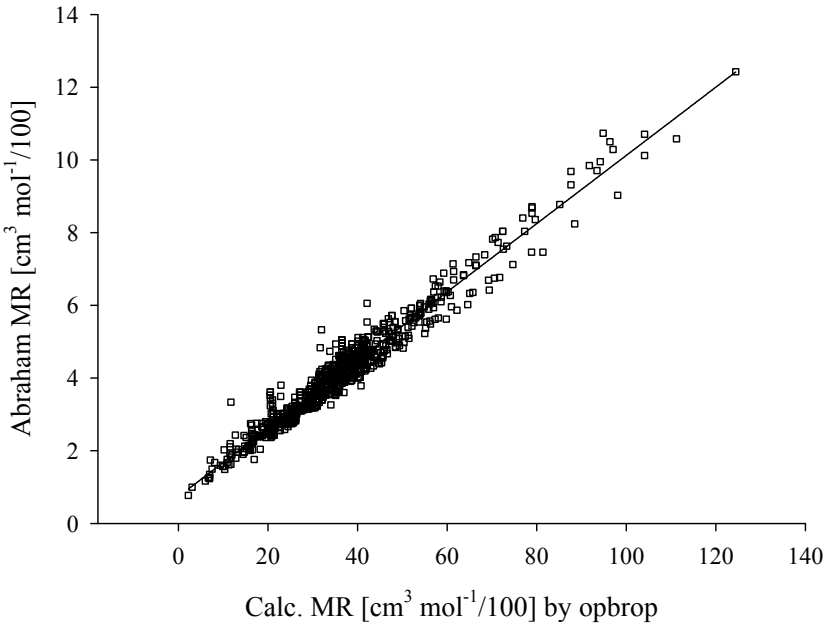


Fig. S2 Correlation between Abraham molecular refraction (MR) and OBPROP molecular refraction (MR_{OBP})

$$\text{Abraham MR [cm}^3\text{ mol}^{-1}\text{/100]} = 0.09406\ MR_{OPB} - 0.3245 \qquad \text{Eq. (S1)}$$

$$R^2=0.958\ SE=0.32$$

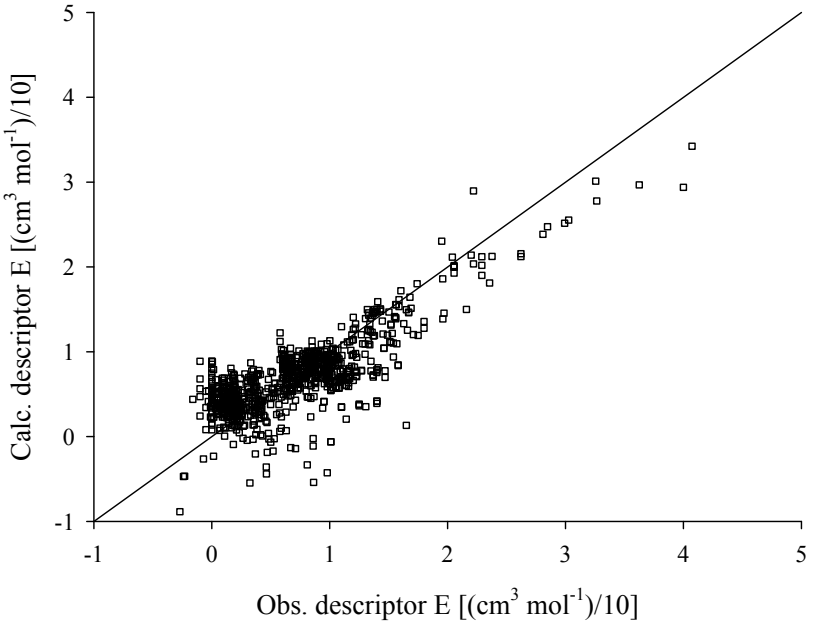


Fig. S3 Correlation between Abraham E and calculated E by Eq. (8)

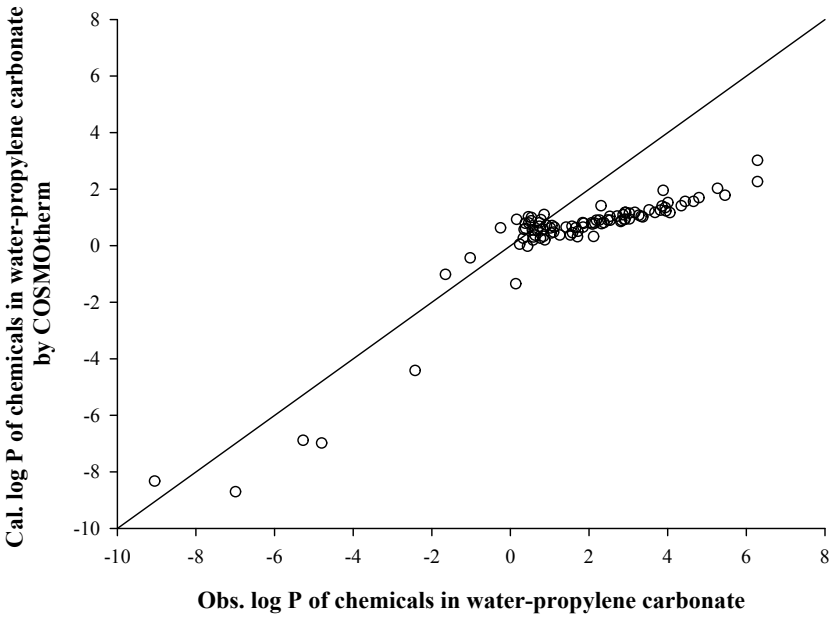


Fig. S4 Correlation between observed and COSMOtherm-calculated log P of chemicals in water-propylene carbonate

Table S1 Calculated (Calc.) and literature (AB) solute descriptors of outliers

	Obs. S	Calc. S	Obs A	Calc. A	Obs B	Calc. B	Obs J^+	Calc. J^+	Obs J^-	Calc. J^-
3-CyanoPy$^+$	1.87	2.73								
4-CyanoPy$^+$	7.16	2.65	4.65	1.99						
4-DimethylaminoPy$^+$	6.71	1.83	3.75	1.16						
morphine$^+$			1.25	2.65			3.94	2.04		
F$^-$					2.42	6.86				
Phthalicacid^{1-}	1.58	3.93			2.03	3.13				
Succinicacid^{2-}					6.24	4.84				
Indomethacin					4.38	2.44				
Meloxicam					4.18	2.69				
Piroxicam					4.18	2.76				
Phentolamine					4.13	2.75				
Naphthoic acid	4.13	6.16								
Bupivacaine			2.92	1.62						
Ropivacaine			2.92	1.52						
Verapamil	7.7	6.09	4.33	1.69						
Donepezil			3.16	1.36						
Rizatriptan			3.82	2.29						
Tacrine	7.24	3.87	5.02	1.95			-0.539	1.366		
Thioridazine			3.33	1.53						
Astemizole$^+$			3.39	1.81						
Amiodaron$^+$	4.95	6.09	2.78	1.02						
2-AcetlyPy$^+$	5.78	1.42	3.89	1.25						
2-BromoPy$^+$			3.5	1.57						
2-ChloroPy$^+$			2.7	1.57						
2,6-Dibromo-nitroPX$^-$	8.7	6.14							3.95	2.38
Ph4B$^-$	2.72	12.52							-0.188	4.29
Tamoxifen$^+$			2.53	0.70					4.15	2.25
Minoxidil							3.94	2.21		
Ph4As+							1.602	0.581		
Quinidine+							4.150	2.244		

Table S2. COSMOtherm-predicted, Calculated by Eq. (24) and observed the transfer of compounds from water to propylene carbonate. The observed data were obtained from ref 1.

Chemical	Obs.	Calc. by Eq. (24)	Cosmotherm-predicted
Hydrogen	0.26	0.26	0.02
Nitrogen	0.60	0.71	0.17
Carbon dioxide	0.71	0.72	0.50
Hydrogen sulfide	0.65	0.63	0.33
Sulfer dioxide	0.85	0.43	0.55
Carbonyl Sulfide	1.14	1.28	0.62
Water	-1.63	0.16	-1.05
Methane	0.86	0.77	0.30
Ethane	1.44	1.23	0.62
Propane	1.87	1.71	0.62
Butane	2.40	2.19	0.78
Pentane	2.92	2.66	0.89
Hexane	3.35	3.15	1.00
Heptane	3.84	3.62	1.22
Octane	4.37	4.10	1.38
Nonane	4.68	4.58	1.53
Dodecane	5.29	5.06	1.99
Isobutane	2.34	2.20	0.75
2-Methylpentane	3.29	3.14	1.04
2,4-Dimethylpentane	3.70	3.62	1.14
2,5-Dimethylhexane	3.96	4.10	1.31
2,3,4-Trimethylpentane	3.98	4.03	1.20
Cyclohexane	2.85	2.74	0.86
Methylcyclopentane	2.94	2.84	0.90
Methylcyclohexane	3.39	3.22	0.98
Ethylcyclohexane	4.08	3.71	1.14
Ethene	1.12	0.83	0.45
Propene	1.69	1.25	0.60
Hex-1-ene	2.89	3.15	1.06
Oct-1-1ene	3.88	3.63	1.37
2-Methylbut-2-ene	2.50	2.19	0.88
1,3-Butadiene	1.89	1.55	0.76
2-Methylbuta-1,3-diene	2.29	1.99	0.87
Cyclohexene	2.56	2.23	0.86
Benzene	2.21	1.97	0.86

Toluene	2.55	2.39	1.00
Ethylbenzene	2.95	2.88	1.14
o-Xylene	3.05	2.80	1.11
m-Xylene	2.94	2.82	1.14
p-Xyelene	2.95	2.83	1.14
Diethyl ether	0.61	1.09	0.27
Diisopropyl ether	1.04	1.96	0.59
Methyl tert-butylether	0.79	1.39	0.23
Ethyl tert-butyl ether	1.06	1.83	0.41
Methyl tert-pentyl ether	1.28	1.83	0.34
Isopropyl tert-butyl ether	1.60	2.37	0.42
Butanone	0.46	0.60	-0.06
Pentan-2-one	0.90	1.04	0.17
Dichloromethane	1.59	1.56	0.65
Trichloromethane	2.09	2.25	0.78
1,2-Dichloroethane	1.86	1.82	0.78
tert-Butyl chloride	2.83	1.99	0.82
tert-Butyl bromide	3.05	2.11	0.91
Iodoethane	2.17	1.61	0.77
Triethylamine	-0.23	2.46	0.60
Tetramethyltin	3.19	3.25	1.14
Biphenyl	4.47	3.92	1.53
Anthracene	4.82	4.48	1.66
Pyrene	5.48	4.94	1.75
Benzil	4.03	3.82	1.49
Monouron	2.11	2.84	0.73
Diuron	2.74	3.56	1.01
Diphenylsulfone	3.55	3.40	1.23
2-Methylbenzoic acid	1.73	1.65	0.29
2-Methoxybenzoic acid	1.55	1.69	0.34
4-Chlorobenzoic acid	2.14	1.89	0.29
4-Nitrobenzoic acid	1.74	1.67	0.47
Anion			--
Cl^-	-6.97	-6.93	-8.74
Br^-	-5.25	-5.45	-6.92
I^-	-2.40	-3.22	-4.45
$ClO4^-$	0.16	-1.86	-1.38
$N3^-$	-4.78	-5.72	-7.02
$Ph4B^-$	6.31	7.09	2.23

$Acetate^-$	-9.03	-8.21	-8.36
$Picrate^-$	-1.00	-0.83	-0.47
Cation			--
$BuNH3^+$	0.35	1.01	0.23
$Et4N^+$	2.33	1.51	1.38
$Pr4N^+$	3.91	2.84	1.92
$2\text{-}MethylPy^+$	0.55	0.34	0.85
$3\text{-}MethylPy^+$	0.40	0.60	0.76
$4\text{-}MethylPy^+$	0.49	0.84	0.77
$2,3\text{-}DimethylPy^+$	0.56	0.92	0.96
$2,4\text{-}DimethylPy^+$	0.48	1.12	0.99
$2,6\text{-}DimethylPy^+$	0.88	0.76	1.07
$3,4\text{-}DimethylPy^+$	0.80	1.25	0.89
$3,5\text{-}DimethylPy^+$	0.18	1.25	0.90
$2\text{-}ChloroPy^+$	0.76	0.78	0.77
$3\text{-}ChloroPy^+$	0.94	1.01	0.69
$3\text{-}CyanoPy^+$	0.58	1.05	0.52
$4\text{-}CyanoPy^+$	0.41	1.24	0.58
$2\text{-}AminoPy^+$	0.37	0.73	0.54
$3\text{-}AminoPy^+$	0.76	0.72	0.65
$4\text{-}AminoPy^+$	1.08	0.87	0.68
$Ph4As^+$	6.31	5.34	2.98

Table S3. Calculated [by Eq. (25)] and observed the transfer of compounds from water to sulfolane. The observed data were obtained in ref 2.

Chemical	Obs.	Calc.
Carbon dioxide	0.55	0.55
Nitrous oxide	0.58	1.13
Sulfer dioxide	0.87	0.58
Hydrogen sulfide	0.77	0.75
Ethane	1.09	1.13
Butane	2.11	2.09
Pentane	2.72	2.55
Hexane	3.23	3.03
Heptane	3.78	3.52
Octane	4.11	4.00
Nonane	4.49	4.48
Dodecane	5.05	4.96
2,2,4-Trimethylpentane	3.83	3.92
Cyclohexane	2.71	2.98
Cycloheptane	2.88	3.48
Cyclooctane	3.43	3.94
Methylcyclopentane	2.79	3.02
Methylcyclohexane	3.23	3.45
1-Butene	1.91	1.62
Isobutene	1.79	1.58
trans-2-Butene	1.97	1.63
cis-2-Butene	2.08	1.59
1,3-Butadiene	1.77	1.47
1-Hexene	2.69	2.56
1-Heptene	3.12	3.04
1-Octene	3.66	3.52
Cyclohexene	2.47	2.47
1-Hexyne	2.61	2.08
1-Heptyne	3.31	2.55
1-Octyne	3.61	3.03
Dichloromethane	1.74	1.57
Chloroform	2.25	2.34
Carbon tetrachloride	2.76	2.96
Chloroethane	1.33	1.08
1,2-Dichloroethane	2.08	1.79

Trichloroethene	2.58	2.73
Acetonitrile	0.46	0.22
Diethyl ether	0.57	0.80
Diisopropyl ether	0.90	1.67
Methyl tert-butyl ether	0.41	1.04
Ethyl tert-butyl ether	0.90	1.49
Tetrahydrofuran	0.16	0.60
Dioxane	-0.27	0.01
Methylformate	0.33	0.30
Methyl acetate	0.37	0.25
Ethyl acetate	0.71	0.47
Propyl acetate	1.12	0.84
Butyl acetate	1.59	1.23
Acetaldehyde	-0.43	0.19
Isobutyraldehyde	0.57	0.79
Acetone	-0.08	0.09
Butanone	0.31	0.30
4-Methyl-2-pentanone	1.18	1.29
Methanol	-0.94	-0.49
Ethanol	-0.70	-0.37
Butan-1-ol	0.25	0.32
2-Propanol	-0.52	-0.06
2-Methyl-1-propanol	0.28	0.58
Allyl alchol	0.01	-0.12
Nitromethane	0.92	0.73
Benzene	2.31	2.25
Toluene	2.62	2.67
Ethylbenzene	2.99	3.14
o-Xylene	3.08	3.08
m-Xylene	2.95	3.10
p-Xyelene	2.93	3.11
Chlorobenzene	2.95	3.03
Pyridine	0.39	0.82
Benzoic acid	1.89	1.51
2-Methylbenzoic acid	2.21	1.82
3-Methylbenzoic acid	2.26	1.83
2-Chlorobenzoic acid	2.19	2.11

4-Chlorobenzoic acid	2.69	2.17
2-Nitrobenzoic acid	1.66	2.28
4-Nitrobenzoic acid	2.74	2.08
Cation		--
$Ph4AS^+$	6.23	6.23
Anion		--
Cl^-	-9.24	-9.52
Br^-	-6.96	-7.32
I^-	-3.59	-3.98
$N3^-$	-6.96	-7.65
$Ph4B^-$	6.23	6.66
$Benzoate^-$	-8.83	-9.33
$3\text{-Methylbenzoate}^-$	-9.10	-9.15
$4\text{-Methylbenzoate}^-$	-9.37	-9.20
$4\text{-tert-Butylbenzoate}^-$	-8.04	-8.14
3-CF3-benzoate^-	-7.69	-8.12
3-Cyanobenzoate^-	-8.74	-8.90
4-Cyanobenzoate^-	-8.49	-8.87
$3\text{-Acetylbenzoate}^-$	-9.25	-9.19
$4\text{-Acetylbenzoate}^-$	-9.14	-9.23
$Terephthalicaicd^-$	-9.01	-8.73
4-Aminobenzoate^-	-10.60	-9.08
3-HO-benzoate^-	-10.81	-9.01
4-Ho-benzoate^-	-10.44	-9.00
3-Meo-benzoate^-	-9.44	-9.15
3-Pho-benzoate^-	-6.70	-6.75
4-Pho-benzoate^-	-5.80	-6.83
3-SH-benzoate^-	-8.46	-8.25
4-SH-benzoate^-	-8.79	-8.37
4-SMe-benzoate^-	-8.84	-8.40
$3\text{-SO2Me-benzoate}^-$	-9.38	-10.00
$4\text{-SO2Me-benzoate}^-$	-9.53	-9.92
$3\text{-So2NH2-benzoate}^-$	-10.14	-9.67
$4\text{-SO2NH2-benzoate}^-$	-10.19	-9.68
$3\text{-Fluorobenzoate}^-$	-9.06	-8.90
$4\text{-Fluorobenzoate}^-$	-9.58	-8.99
$3\text{-Chlorobenzoate}^-$	-8.16	-8.43
$4\text{-Chlorobenzoate}^-$	-8.03	-8.46

3-Bromobenzoate$^-$	-7.53	-8.13
4-Bromobenzoate$^-$	-7.67	-8.15
3-Iodobenzoate$^-$	-7.07	-7.71
4-Iodobenzoate$^-$	-7.42	-8.28
3-Nitrobenzoate$^-$	-8.47	-8.42
4-Nitrobenzoate$^-$	-7.79	-8.39

Table S4. Calculated [by Eq. (26)] and observed the transfer of compounds from water to ethylene glycol. The observed data were obtained in ref 1.

Chemical	Obs.	Calc.
1,4-Dioxane	3.27	3.75
1-nitronaphthalene	6.65	6.91
2,3,4-Trimethylpentane	0.77	1.48
2,4,4-trimethyl-1-pentene	1.08	1.79
2-hydroxybenzoic acid	7.43	7.87
2-Methylbuta-1,3-diene	0.82	1.17
2-Methylpropane	0.14	0.19
2-Nitrophenol	5.02	5.35
3-Chlorophenol	7.37	4.81
3-methyl-1-butene	0.56	1.02
4-Ethylphenol	6.55	5.16
4-hydroxybenzoic acid	8.53	8.46
Acenaphthene	5.22	5.95
Acetanilide	8.02	6.18
Ammonia	2.25	-0.44
Aniline	5.52	4.29
anisole	3.23	3.37
Anthracene	6.57	6.67
Benzene	2.03	2.09
Benzoic acid	6.86	5.97
Benzonitrile	4.26	3.81
Benzyl alcohol	6.09	4.93
Biphenyl	5.23	5.18
Bromobenzene	3.22	3.05
Buta-1,3-diene	0.99	0.81
Butanone	2.64	2.45
Carbon dioxide	0.10	-0.39
cis-2-hexene	0.91	1.42
Cyclohexane	1.13	1.53
Cyclohexene	1.39	2.18
Ethane	-0.63	-0.48
Ethanol	3.48	2.11
Ethene	-0.37	-0.08
Ethylbenzene	2.49	2.84

Ethylcyclohexane	1.52	2.17
Ethyne	0.50	0.25
Fluoranthrene	7.50	7.98
Fluorene	5.73	6.24
Hept-1-ene	1.07	1.76
hexafluorobenzene	1.16	1.09
Hydrogen	-1.75	-1.56
ibuprofen	8.97	7.98
Isopropylbenzene	2.59	3.15
Methane	-1.14	-0.86
methyl-4-hydroxybenzoate	8.58	7.90
Methylcyclohexane	1.20	1.84
m-Xylene	2.51	2.94
Naphthalene	4.27	4.40
naproxen	11.79	10.23
n-Butane	0.21	0.21
n-Decane	1.97	2.29
n-Heptane	0.85	1.25
n-Hexane	0.56	0.82
Nitrobenzene	4.44	4.33
Nitrogen	-1.81	-0.76
Nitromethane	3.09	2.53
Nitrous oxide	-0.13	-1.14
n-Nonane	1.43	1.94
n-Octane	1.14	1.59
n-Propylbenzene	2.68	3.19
Oct-1-ene	1.33	2.10
o-Xylene	2.67	2.94
Phenanthrene	6.28	6.71
Phenol	6.39	4.39
Propane	0.03	-0.13
Propene	0.33	0.36
p-Xylene	2.49	2.93
Pyrene	7.62	8.18
Tetramethyltin	0.90	0.51
Toluene	2.35	2.52
trans-2-hexene	0.79	1.38

trans-Stilbene	6.30	6.09
Anion		--
2-Aminobenzoate$^-$	-1.27	-0.45
2-Chlorobenzoate$^-$	-0.92	-0.77
2-Nitrobenzoate$^-$	-1.35	-0.02
3-Chlorobenzoate$^-$	-0.37	-0.82
3-Hydroxylbenzoate$^-$	-0.90	0.26
3-Nitrobenzoate$^-$	-0.70	0.64
4-Aminobenzoate$^-$	-1.55	-1.41
4-Chlorobenzoate$^-$	-0.26	-0.96
4-hydroxybenzoate$^-$	-0.97	0.20
4-Nitrobenzoate$^-$	-0.77	0.60
Acetate$^-$	-2.42	-4.15
Benzoate$^-$	-1.23	-1.49
Br^-	-1.62	-2.97
Chloroacetate$^-$	-1.89	-1.61
Cl^-	-2.07	-5.65
I^-	-1.10	1.25
$Ph4B^-$	3.60	2.42
Phenylacetate$^-$	-1.31	-1.13
Cation		--
$Et2NH2^+$	-0.07	0.81
$Et3NH^+$	0.06	-0.76
$EtNH3^+$	-0.15	1.59
$Me2NH2^+$	-0.50	0.77
$Me3NH^+$	-0.35	-1.38
$MeNH3^+$	-0.32	1.64
$Ph4AS^+$	3.60	2.53

References

1. M. H. Abraham, W. E. Acree Jr, *New J. Chem.* 2010, **34**, 2298-2305.
2. T. W. Stephens, N. E. Rosa, M. Saifullah, S. Ye, V. Chou, A. N. Quay, W. E. Acree Jr., M. H. Abraham, *Fluid Phase Equilib.* 2011, **309**, 30-35.