Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

A simple COSMO-based method for calculation of hydration energies of neutral molecules

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Supporting information

Table S1. Optimized parameters κ_A, g_A and h_A for elements H, C–F, P–Cl, Br, and I, for various atomic-charge and radii choices.

	H	C	N	O	F	P	S	Cl	Br	I
					Bondi radii, CM5 charges: f= 1.15					
κ_A	0.0234	0.0269	0.0112	-0.0094	0.0371	0.1317	-0.0267	-0.0041	-0.0201	-0.028
g_A	0.78	-0.82	3.16	8.34	11.43	-33.0	4.03	3.46	4.08	5.57
h_A	48.2			16.9						
					Bondi radii, ACP charges: f= 1.15					
κ_A	0.0315	0.0175	0.0132	-0.0109	0.0242	0.1888	0.0144	-0.0026	-0.0004	-0.0109
g_A	0.3552	2.2811	6.6842	14.1486	22.3078	39.3410	3.8988	9.6626	11.0529	10.5591
h_A	144.5614			31.9229						
					UFF radii, CM5 charges: f = 1.342					
κ_A	0.0111	0.0333	0.0484	-0.0093	0.0306	0.0284	-0.0294	-0.0065	-0.0122	-0.0274
g_A	1.5463	-4.58	-7.33	2.88	12.37	2.81	8.64	5.26	1.49	11.52
h_A	113.28			2.12						
					UFF radii, ESP charges: f = 1.2947					
κ_A	0.0269	0.0076	0.0652	-0.0165	0.0429	0.0646	-0.0006	-0.0028	-0.0136	-0.0214
g_A	3.1529	5.3097	0.6640	4.385	9.4668	-4.2772	7.9391	6.5522	1.7820	1.3770
h_A	18.1277			-16.0993						
					UFF radii, ACP charges: f = 0.7736					
κ_A	0.0093	0.0194	0.0016	-0.0091	0.0274	0.0479	0.0377	-0.0061	0.0109	-0.0127
g_A	0.0043	-2.3864	-7.7931	1.6047	21.0567	1.0780	0.8402	12.2381	6.8475	14.9273
h_A	326.2373			9.7427						

Table S2. Mean signed error (MSE), mean absolute error (MAE), and standard deviation (SD) of the solvation free energy calculated by various methods with respect to the reference values in kcal·mol^{-1} (Bondi radii).

Dataset		Solvation scheme					
		SSE-ACP	SSE-I-ACP	SSE-CM5	SSE-ESP	SMD[b]	PCM[b]
All molecules(390)[a]	MSE	-0.16	0.04	-0.08	-0.05	0.57	0.31
	MAE	1.09	1.23	0.94	1.13	1.15	1.85
	SD	1.56	1.78	1.50	1.62	1.69	2.34
Small molecules(24)[c]	MSE	-0.88	-0.82	-0.56	-0.53	-0.05	-0.88
	MAE	0.99	1.23	0.61	0.86	0.45	1.45
	SD	1.27	1.53	0.84	1.27	0.62	1.75
Alcohols(18)	MSE	0.89	0.44	0.28	0.60	0.82	1.88
	MAE	0.89	0.52	0.43	0.69	0.82	1.88
	SD	1.11	0.76	0.66	0.84	0.86	2.03
Aldehydes and ketones(22)	MSE	-0.47	0.30	0.44	-0.26	0.27	0.12
	MAE	0.68	0.37	0.50	0.48	0.49	1.05
	SD	0.91	0.55	0.63	0.58	0.77	1.47
Ethers(10)	MSE	-0.12	1.00	0.02	0.67	0.91	0.17
	MAE	0.48	1.12	0.44	0.97	1.01	0.61
	SD	0.58	1.31	0.56	1.13	1.10	0.87
Esters(21)	MSE	-0.24	-0.13	-0.33	-0.99	0.52	0.07
	MAE	0.88	0.41	0.56	1.14	0.59	1.20
	SD	1.28	0.45	0.70	1.28	0.84	1.49
Acids(10)	MSE	0.37	0.28	-0.08	0.22	1.82	2.79
	MAE	0.51	0.84	0.24	0.50	1.82	2.79
	SD	0.65	0.92	0.33	0.58	2.01	2.91
Amines(42)	MSE	0.56	0.74	0.33	0.69	0.81	2.16
	MAE	1.32	1.31	1.27	1.26	0.88	2.16
	SD	1.61	1.71	1.54	1.72	0.96	2.49
Nitriles(4)	MSE	-2.62	-2.75	-1.55	-2.78	0.22	-1.28
	MAE	2.62	2.75	1.55	2.78	0.27	1.28
	SD	2.74	2.87	1.70	2.80	0.37	1.30
Nitro compounds and nitrates(17)							
MSE		-0.56	0.05	-0.18	-0.24	1.36	-0.81
	MAE	1.05	1.06	0.88	0.96	1.74	1.57
	SD	1.49	1.43	1.16	1.31	2.10	1.80
Fluorine compounds(33)							
	MSE	0.11	-0.09	0.26	-0.01	0.31	-1.78
	MAE	1.16	0.99	1.04	0.81	1.07	2.63
	SD	1.44	1.32	1.43	1.15	1.48	2.98
Chlorine compounds(74)							
	MSE	-0.26	0.07	0.14	0.31	0.81	0.03
	MAE	1.17	1.23	0.95	1.12	1.68	1.73
	SD	1.64	1.86	1.55	1.63	2.27	2.35
Bromine compounds(25)							
	MSE	0.12	0.14	-0.01	0.18	0.31	-0.34
	MAE	0.68	0.92	0.36	0.88	0.96	1.61
	SD	0.89	1.25	0.78	1.26	1.60	2.22
Iodine compounds(10)							
	MSE	0.06	0.12	0.05	0.06	0.13	-0.30
	MAE	0.58	0.90	0.55	0.78	0.81	2.02
	SD	1.07	1.70	1.00	1.33	1.34	3.05
Worst ACP cases(10)	MSE	-3.77	-5.70	-5.07	-4.09	-4.01	-1.18
	MAE	4.51	5.70	5.07	4.09	4.01	1.84
	SD	4.57	6.11	5.79	4.73	4.90	2.19
Worst SMD cases(10)	MSE	0.86	-1.28	-1.05	-0.11	0.27	2.21
	MAE	2.34	4.94	4.13	3.91	5.77	3.51
	SD	3.05	5.63	4.97	4.46	5.99	4.48
Best ACP cases(380)	MSE	-0.03	0.19	0.05	0.05	0.69	0.35
	MAE	0.98	1.11	0.84	1.06	1.07	1.85
	SD	1.29	1.51	1.19	1.45	1.52	2.34
Linear correlation[d] (for all molecules)							
Slope		0.95	0.93	0.99	0.94	0.92	0.57
Intercept		-0.39	-0.29	-0.12	-0.34	0.23	-1.58
R^2		0.88	0.85	0.90	0.87	0.87	0.78
		ACP	I-ACP	CM5	ESP	SMD[b]	PCM[b]

[a] The complete list of molecules for all the subsets is given in the Supporting Information.
[b] Calculated using the Gaussian program package.
[c] Molecules containing less than six atoms.
[d] Linear correlation between reference solvation free energy and that calculated within a given solvation method.

Table S3. Data subset composition. The codes of the molecules correspond to those in the Minnesota Solvation Database.[1]

Dataset	**Molecules**
Small molecules(24)	0001met, 0030eth, 0153flu, 0160chl, 0161dic, 0162tri, 0177bro, 0178dib, 0179tri, 0197bro, 0198chl, 0199chl, 0200tet, 0216amm, 0217wat, 0218pho, 0219hyd, 0400hyd, 0421dfl, 0422ftc, 0423brt, n017, test4002, test4003
Alcohols(18)	0044met, 0045eth, 0046eth, 0047pro, 0048pro, 0049but, 0050met, 0051cyc, 0052pen, 0053phe, 0054hex, 0055ocr, 0056mcr, 0057pcr, 0058hep, 0145pro, 0146met, 0236oct
Aldehydes and ketones(22)	0070eth, 0071proa, 0072but, 0073pen, 0074ben, 0145pro, 0150mhy, 0151phy, 0237oct, test2001, 0075pro, 0076but, 0077cyc, 0078pen, 0079pen, 0080hex, 0081dim, 0082hep, 0083hep, 0084met, 0085non, 0239oct
Ethers(10)	0060dim, 0063die, 0064met, 0065met, 0067but, 0242dii, 0246eth, 0062dio, 0068ani, 0061tet
Esters(21)	0091met, 0092ethb, 0093met, 0094met, 0095eth, 0096met, 0097pro, 0098met, 0099but, 0100met, 0101pen, 0238met, 0240met, test0011, test0013, test0016, test2003, test2011, test2020, test2026, test0013
Acids(10)	test2021, 0086eth, 0087pro, 0088but, 0089pen, 0090hex, test2001, test3007, test3014, test3015
Amines(42)	0103eth, 0104dim, 0105aze, 0106pro, 0107tri, 0108pyr, 0109pip, 0110but, 0111die, 0112Nme, 0113pen, 0114NNd, 0115dip, 0116pyr, 0117met, 0118ani, 0119met, 0120met, 0121met, 0122Nme, 0123dim, 0124dim, 0125dim, 0216amm, 0225pipa, 0228met, 0229hyd, 0230eth, 0402adn, 0471dim, 0571dim, 0574eth, n005, n006, n009, n010, n011, n013, n014, n015, n016, test0017
Nitriles(4)	0126eth, 0127pro, 0128butb, 0129ben
Nitro compounds and nitrates(17)	0130nit, 0131nit, 0132nit, 0133nit, 0134nit, 0135met, 0506nit, test1001, test1002,test1028, test1041, test1058, test2022, test1003, test1004, test1005, test1006
Fluorine compounds(33)	0153flu, 0154dif, 0157flu, 0197bro, 0198chl, 0199chl, 0200tet, 0201bro, 0203bro, 0205chl, 0206tri, 0207tri, 0209chl, 0211tri, 0212hex, 0214tri, 0405hex, 0406oct, 0421dfl, 0422ftc, 0424clp, n200, n201, test0004, test1011, test1027, test1046, test1056, test2010, test2013, test2023, test2029, test3021
Chlorine compounds(74)	0160chl, 0161dic, 0162tri, 0163chl, 0165tri, 0166tri, 0167chla, 0168chl, 0169chl, 0170chl, 0171Zdi, 0172Edi, 0173tri, 0174chl, 0175odi, 0176pdi, 0198chl, 0199chl, 0201bro, 0202bro, 0204tet, 0205chl, 0206tri, 0209chl, 0213bis, 0407tet, 0408hex, 0409clb, 0410clp, 0411chp, 0412clt, 0413clt, 0414dcl, 0415dcl, 0416dcl,

	0421dfl, 0422ftc, 0423brt, 0424clp, 0426dcl, 0427dcl, 0428ami, 0433pho, 0438pho, 0440pho, 0442pho, 0444pho, 0445pho, n202, test0007, test1007, test1014, test1017, test1018, test1019, test1020, test1021, test1022, test1023, test1025, test1029, test1030, test1033, test1035, test1048, test1049, test1050, test1052,test1055, test2006, test2015, test2024, test3019, test3020
Bromine compounds(25)	0177bro, 0178dib, 0179tri, 0180bro, 0182bro, 0183bro, 0184bro, 0185bro, 0186bro, 0187dib, 0197bro, 0201bro, 0202bro, 0203bro, 0215pbr, 0417brp, 0418bri, 0419brt, 0420pbr, 0423brt, 0425dbr, 0442pho, 0445pho, n203, test1013
Iodine compounds(10)	0939tet, test2018, test4001, test4002, test4003, test4004, test4006, test4007, test4008, test4009
Worst ACP cases(10)	0126eth, test1060, test1039, 0437pho, test1040, test1054, test1023, c000, test1029, test1012
Worst SMD cases(10)	n203, test1001, test1025, test1029, test1049, test2006, test1039, test1054, test2024, test1012

Table S4. Hydration free energies for the 390-molecule dataset in kcal·mol^{-1}. The codes of the molecules correspond to those in the Minnesota Solvation Database.[1]

Code	Name	exper.	ESE-ACP	ESE-CM5	ESE-IACP	ESE-ESP	SMD	PCM
0001met	methane	2.0	0.6	0.8	-0.0	0.5	2.2	-0.1
0002eth	ethane	1.8	0.8	0.9	0.4	1.2	1.8	-0.1
0003pro	n-propane	2.0	1.0	1.1	0.6	1.3	1.8	-0.1
0004nbu	n-butane	2.1	1.2	1.2	0.8	1.5	2.0	-0.2
0005npe	n-pentane	2.3	1.4	1.3	1.0	1.8	2.2	-0.2
0006nhe	n-hexane	2.5	1.5	1.4	1.1	2.1	2.4	-0.2
0007nhe	n-heptane	2.6	1.7	1.6	1.3	2.3	2.5	-0.3
0008noc	n-octane	2.9	-0.4	0.8	1.5	2.7	2.7	-0.3
0010met	2-methylpropane	2.3	1.2	1.2	0.6	1.2	2.0	-0.2
0011dim	2,2-dimethylpropane	2.5	1.5	1.5	0.7	1.2	2.2	-0.3
0012met	2-methylpentane	2.5	1.6	1.6	1.0	1.8	2.4	-0.2
0013dim	2,4-dimethylpentane	2.9	1.9	1.8	1.1	1.7	2.6	-0.3
0014tri	2,2,4-trimethylpentane	2.9	2.1	2.0	1.1	1.7	2.7	-0.4
0016cyc	cyclopropane	0.8	0.1	0.5	-0.1	-0.1	0.1	-0.6
0017cyc	cyclopentane	1.2	1.1	1.0	1.0	1.9	1.3	-0.2
0018cyc	cyclohexane	1.2	1.5	1.3	1.2	2.1	1.4	-0.1
0019met	methylcyclohexane	1.7	1.7	1.4	1.3	2.0	1.8	-0.2
0020cis	cis-1,2-dimethylcyclohexane	1.6	2.0	1.7	1.3	2.1	2.0	-0.2
0021eth	ethene	1.3	-0.3	0.3	-0.6	-1.1	1.4	-0.8
0022pro	propene	1.3	-0.1	0.3	-0.4	-0.6	1.2	-0.8
0023str	s-trans-1,3-butadiene	0.6	-0.7	0.0	-0.9	-1.6	0.9	-1.3
0024met	2-methylpropene	1.2	0.2	0.3	-0.4	-0.4	1.3	-0.9
0025buta	1-butene	1.4	0.0	0.4	-0.2	-0.0	1.2	-0.8
0026cyc	cyclopentene	0.6	-0.1	0.1	0.1	0.6	0.5	-0.6
0027pen	1-pentene	1.7	0.3	0.6	-0.0	-0.0	1.4	-0.8
0028Epe	E-2-pentene	1.3	0.5	0.6	0.3	0.5	1.4	-0.7
0029hex	1-hexene	1.7	0.6	0.9	0.3	0.4	1.6	-0.9
0030eth	ethyne	-0.0	-2.8	-1.1	-4.1	-4.4	-0.2	-2.2
0031pro	propyne	-0.3	-2.2	-1.2	-3.7	-3.1	-0.5	-2.1
0032but	1-butyne	-0.2	-1.6	-0.7	-3.1	-2.5	-0.2	-2.1
0033pen	1-pentyne	0.0	-1.3	-0.5	-2.6	-2.1	-0.0	-2.0
0034hex	1-hexyne	0.3	-1.0	-0.3	-2.7	-2.1	-0.0	-2.2
0035ben	benzene	-0.9	-2.0	-1.2	-1.2	-1.7	-0.7	-1.6
0036tol	toluene	-0.9	-1.4	-1.0	-1.0	-1.0	-0.3	-1.6
0037eth	ethylbenzene	-0.8	-1.1	-0.8	-0.7	-0.6	-0.1	-1.7
0038oxy	o-xylene	-0.9	-1.0	-1.0	-0.9	-1.0	-0.3	-1.7
0039mxy	m-xylene	-0.8	-0.9	-0.9	-0.8	-0.7	0.1	-1.6
0040pxy	p-xylene	-0.8	-0.8	-0.9	-0.8	-0.7	0.1	-1.6
0041nap	naphthalene	-2.4	-2.5	-1.9	-1.6	-2.1	-1.5	-2.3
0042ant	anthracene	-4.2	-3.1	-2.5	-1.9	-2.6	-2.2	-2.9
0044met	methanol	-5.1	-5.0	-5.3	-5.2	-5.1	-4.2	-3.2
0045eth	ethanol	-5.0	-4.8	-5.2	-5.0	-4.5	-4.2	-3.1
0046eth	1,2-ethanediol	-9.3	-8.9	-9.2	-9.0	-7.9	-8.7	-5.2
0047pro	1-propanol	-4.8	-4.2	-4.8	-4.6	-4.7	-4.1	-3.1
0048pro	isopropanol	-4.8	-3.3	-4.0	-4.1	-4.6	-4.3	-3.1
0049but	1-butanol	-4.7	-4.1	-4.7	-4.4	-4.4	-3.9	-3.1

0050met	t-butanol	-4.5	-2.9	-3.7	-4.1	-4.1	-3.8	-3.0
0051cyc	cyclopentanol	-5.5	-2.6	-3.3	-3.1	-3.6	-4.8	-3.0
0052pen	1-pentanol	-4.5	-3.4	-4.1	-4.0	-3.8	-4.0	-3.3
0053phe	phenol	-6.6	-5.8	-6.3	-6.3	-5.4	-5.2	-4.0
0054hex	1-hexanol	-4.4	-3.2	-4.0	-3.8	-3.6	-3.8	-3.3
0055ocr	o-cresol	-5.9	-5.4	-6.0	-6.0	-5.5	-4.6	-3.7
0056mcr	m-cresol	-5.5	-5.3	-6.2	-6.0	-6.0	-4.8	-4.0
0057pcr	p-cresol	-6.1	-5.2	-6.1	-6.0	-5.2	-4.8	-3.9
0058hep	1-heptanol	-4.2	-3.1	-3.9	-3.7	-3.2	-3.6	-3.3
0060dim	dimethylether	-1.9	-2.8	-2.6	-1.2	-1.4	-0.6	-1.8
0061tet	tetrahydrofuran	-3.5	-2.7	-2.4	-1.1	-1.2	-2.1	-2.1
0062dio	1,4-dioxane	-5.0	-5.2	-4.7	-2.6	-3.4	-4.6	-3.2
0063die	diethylether	-1.8	-2.0	-1.9	-1.0	-1.3	-1.2	-1.9
0064met	methylpropylether	-1.7	-1.9	-1.9	-0.6	-0.6	-0.5	-1.8
0065met	methylisopropylether	-2.0	-2.0	-2.0	-1.0	-1.0	-0.6	-1.8
0066dim	1,2-dimethoxyethane	-4.8	-4.2	-4.2	-1.2	-2.5	-2.0	-2.7
0067but	t-butylmethylether	-2.2	-1.2	-1.3	-1.1	-1.3	-0.5	-1.8
0068ani	anisole	-2.5	-3.1	-2.9	-1.9	-3.0	-1.5	-2.7
0070eth	acetaldehyde	-3.5	-5.3	-3.7	-3.6	-4.2	-3.2	-3.7
0071proa	propanal	-3.4	-5.1	-3.4	-3.3	-3.4	-3.1	-3.6
0072but	butanal	-3.2	-4.3	-3.0	-2.8	-3.5	-3.0	-3.7
0073pen	pentanal	-3.0	-4.6	-3.0	-2.9	-3.2	-2.8	-3.6
0074ben	benzaldehyde	-4.0	-5.6	-4.0	-3.3	-5.4	-3.7	-4.1
0075pro	acetone	-3.9	-4.5	-3.6	-4.2	-4.7	-4.1	-4.2
0076but	2-butanone	-3.6	-4.2	-3.2	-3.7	-4.3	-3.8	-3.9
0077cyc	cyclopentanone	-4.7	-3.9	-3.0	-3.3	-4.3	-4.7	-4.2
0078pen	2-pentanone	-3.5	-3.6	-2.8	-3.4	-4.0	-3.7	-4.0
0079pen	3-pentanone	-3.4	-3.9	-2.7	-3.4	-3.3	-3.5	-3.7
0080hex	2-hexanone	-3.3	-3.6	-2.7	-3.3	-4.0	-3.5	-4.0
0081dim	3,3-dimethylbutanone	-2.9	-2.7	-2.3	-3.1	-3.7	-3.2	-3.7
0082hep	2-heptanone	-3.0	-3.4	-2.6	-3.1	-3.5	-3.4	-4.1
0083hep	4-heptanone	-2.9	-2.7	-2.0	-2.7	-3.3	-3.2	-3.8
0084met	acetophenone	-4.6	-4.6	-3.6	-3.9	-4.5	-4.3	-4.3
0085non	5-nonanone	-2.7	-2.7	-1.9	-2.4	-3.1	-2.9	-3.9
0086eth	acetic acid	-6.7	-7.3	-7.4	-7.5	-7.0	-5.7	-4.5
0087pro	propanoic acid	-6.5	-6.6	-6.8	-7.2	-7.0	-5.5	-4.3
0088but	butanoic acid	-6.4	-6.1	-6.4	-6.9	-6.8	-5.4	-4.3
0089pen	pentanoic acid	-6.2	-6.0	-6.3	-6.7	-6.4	-5.3	-4.4
0090hex	hexanoic acid	-6.2	-5.8	-6.2	-6.5	-6.2	-5.1	-4.4
0091met	methyl formate	-2.8	-5.8	-4.6	-3.4	-4.3	-2.2	-3.6
0092ethb	ethyl formate	-2.6	-5.2	-4.0	-3.1	-4.4	-2.4	-3.6
0093met	methyl acetate	-3.3	-4.0	-4.0	-3.7	-4.6	-2.9	-3.7
0094met	methyl propanoate	-2.9	-3.3	-3.4	-3.6	-3.9	-2.7	-3.5
0095eth	ethyl acetate	-3.1	-3.4	-3.4	-3.5	-4.5	-3.1	-3.7
0096met	methyl butanoate	-2.8	-2.9	-3.0	-3.1	-4.3	-2.6	-3.6
0097pro	propyl acetate	-2.9	-2.9	-3.0	-3.2	-4.7	-3.0	-3.8
0098met	methyl pentanoate	-2.6	-2.8	-2.9	-3.0	-4.1	-2.4	-3.6
0099but	butyl acetate	-2.5	-2.8	-2.9	-3.0	-4.2	-2.9	-3.8
0100met	methyl hexanoate	-2.5	-2.6	-2.8	-2.8	-3.9	-2.2	-3.6
0101pen	pentyl acetate	-2.5	-2.6	-2.7	-2.8	-4.0	-2.7	-3.8
0103eth	ethylamine	-4.5	-2.9	-3.6	-4.3	-4.5	-3.8	-2.8
0104dim	dimethylamine	-4.3	-2.8	-3.1	-2.8	-2.6	-3.2	-2.0
0105aze	azetidine	-5.6	-3.3	-3.5	-3.0	-2.5	-4.7	-2.1
0106pro	propylamine	-4.4	-2.6	-3.5	-4.1	-3.8	-3.7	-2.8
0107tri	trimethylamine	-3.2	-2.2	-2.1	-1.1	-0.9	-2.5	-1.3
0108pyr	pyrrolidine	-5.5	-2.7	-2.9	-2.8	-3.1	-5.0	-2.4
0109pip	piperazine	-7.4	-5.6	-6.7	-5.5	-5.2	-8.1	-3.4
0110but	butylamine	-4.3	-2.5	-3.4	-4.0	-3.9	-3.5	-2.8
0111die	diethylamine	-4.1	-1.6	-1.9	-2.2	-2.6	-3.0	-2.0
0112Nme	N-methylpiperazine	-7.8	-5.2	-5.7	-4.0	-4.1	-7.2	-2.8
0113pen	pentylamine	-4.1	-2.7	-3.4	-3.7	-3.6	-3.3	-2.9
0114NNd	N,N'-dimethylpiperazine	-7.6	-4.6	-4.7	-2.3	-1.8	-6.2	-2.2
0115dip	dipropylamine	-3.7	-1.0	-1.5	-1.8	-2.2	-2.6	-2.0
0116pyr	pyridine	-4.7	-5.8	-4.3	-3.8	-4.6	-4.2	-3.2
0117met	2-methylpyrazine	-5.6	-7.1	-5.6	-5.2	-5.2	-6.0	-3.5
0118ani	aniline	-5.5	-5.7	-6.7	-6.3	-5.9	-4.8	-4.1
0119met	2-methylpyridine	-4.6	-4.8	-3.8	-3.6	-4.0	-3.6	-3.0
0120met	3-methylpyridine	-4.8	-5.0	-4.0	-3.7	-4.2	-4.0	-3.3
0121met	4-methylpyridine	-4.9	-5.2	-4.2	-3.8	-4.3	-4.2	-3.4
0122Nme	N-methylaniline	-4.7	-4.8	-5.2	-4.3	-4.1	-3.9	-3.4
0123dim	2,4-dimethylpyridine	-4.9	-4.0	-3.7	-3.4	-4.3	-3.5	-3.2
0124dim	2,5-dimethylpyridine	-4.7	-4.0	-3.6	-3.5	-3.8	-3.4	-3.1
0125dim	2,6-dimethylpyridine	-4.6	-3.8	-3.3	-3.4	-4.0	-3.0	-2.8
0126eth	acetonitrile	-3.9	-7.7	-6.4	-7.5	-7.2	-4.0	-5.4
0127pro	propionitrile	-3.9	-6.5	-5.5	-6.9	-6.5	-3.7	-5.2
0128butb	butanonitrile	-3.6	-6.1	-5.2	-6.6	-6.0	-3.5	-5.0
0129ben	benzonitrile	-4.1	-5.7	-4.6	-5.5	-6.9	-3.4	-5.0
0130nit	nitroethane	-3.7	-5.7	-4.6	-4.5	-4.8	-3.8	-5.0
0131nit	1-nitropropane	-3.3	-4.8	-4.0	-4.0	-4.6	-3.7	-5.0
0132nit	2-nitropropane	-3.1	-4.1	-3.7	-3.8	-4.0	-2.9	-4.6
0133nit	1-nitrobutane	-3.1	-4.7	-3.8	-3.8	-4.3	-3.6	-5.0

0134nit	nitrobenzene	-4.1	-3.7	-3.1	-2.7	-4.1	-2.3	-4.5
0135met	2-methyl-1-nitrobenzene	-3.6	-2.8	-2.6	-2.4	-4.0	-2.2	-4.4
0136met	methanethiol	-1.2	-1.8	-1.2	-0.7	-2.1	-0.8	-2.1
0137ethb	ethanethiol	-1.3	-1.3	-0.8	-0.4	-1.6	-1.0	-2.1
0138pro	1-propanethiol	-1.1	-0.9	-0.6	-0.1	-1.5	-0.9	-2.2
0139thi	thiophenol	-2.5	-2.5	-2.5	-1.0	-2.5	-2.1	-2.8
0140dim	dimethylsulfide	-1.5	-1.6	-0.6	-0.6	-1.5	-0.3	-2.1
0141dim	dimethyldisulfide	-1.8	-1.8	-1.2	-0.6	-1.2	-1.1	-2.4
0142die	diethylsulfide	-1.4	-1.1	-0.2	-0.3	-0.8	-0.2	-2.0
0143dip	dipropylsulfide	-1.3	-0.2	0.3	0.3	-1.2	-0.1	-2.2
0144thi	thioanisole	-2.7	-2.7	-2.0	-1.3	-3.3	-1.8	-2.9
0145pro	allyl alcohol	-5.1	-4.2	-4.4	-4.7	-5.4	-3.9	-3.1
0146met	2-methoxyethanol	-6.8	-6.5	-7.0	-5.4	-6.1	-6.1	-4.3
0147met	2-methoxyethanamine	-6.5	-5.6	-6.4	-5.3	-5.8	-5.8	-4.2
0148but	butenyne	0.0	-2.1	-0.9	-3.2	-3.2	0.2	-2.1
0149mor	morpholine	-7.2	-5.3	-5.7	-4.0	-4.1	-6.5	-3.4
0150mhy	m-hydroxybenzaldehyde	-9.5	-9.7	-9.2	-8.6	-9.2	-8.1	-6.4
0151phy	p-hydroxybenzaldehyde	-10.4	-10.3	-9.8	-9.2	-9.5	-8.7	-6.8
0153flu	fluoromethane	-0.2	-0.5	-0.3	-0.7	-0.4	-0.1	-1.9
0154dif	1,1-difluoroethane	-0.1	-0.1	0.1	-0.8	-0.4	-1.2	-2.5
0157flu	fluorobenzene	-0.8	-0.1	-0.1	-0.2	-1.2	-0.5	-1.9
0160chl	chloromethane	-0.6	-1.9	-1.0	-1.3	-1.2	-0.7	-1.8
0161dic	dichloromethane	-1.4	-3.6	-1.8	-2.2	-1.8	-1.8	-2.2
0162tri	chloroform	-1.1	-3.3	-1.5	-2.2	-1.7	-1.0	-1.7
0163chl	chloroethane	-0.6	-1.3	-0.7	-1.0	-0.6	-0.9	-1.9
0165tri	1,1,1-trichloroethane	-0.2	-0.7	-0.7	-1.3	-0.8	-0.7	-1.6
0166tri	1,1,2-trichloroethane	-1.9	-3.8	-1.9	-2.7	-2.2	-2.8	-2.6
0167chla	1-chloropropane	-0.3	-0.7	-0.4	-0.6	-0.4	-0.9	-1.9
0168chl	2-chloropropane	-0.2	-0.7	-0.3	-0.8	-0.5	-0.8	-1.9
0169chl	chloroethene	-0.6	-1.3	-0.5	-0.8	-1.4	0.2	-1.4
0170chl	3-chloropropene	-0.6	-2.2	-1.0	-1.5	-1.6	-0.9	-2.1
0171Zdi	Z-1,2-dichloroethene	-1.2	-2.8	-1.3	-1.5	-1.5	-0.6	-1.9
0172Edi	E-1,2-dichloroethene	-0.8	-1.4	-0.8	-0.7	-1.1	-0.0	-1.4
0173tri	trichloroethene	-0.4	-1.0	-0.6	-0.7	-0.5	0.7	-1.2
0174chl	chlorobenzene	-1.1	-1.4	-1.2	-0.7	-1.3	-0.9	-1.8
0175odi	1,2-dichlorobenzene	-1.4	-1.1	-1.0	-0.7	-0.9	-0.8	-2.0
0176pdi	1,4-dichlorobenzene	-1.0	-0.8	-1.0	-0.4	-0.9	-0.9	-1.8
0177bro	bromomethane	-0.8	-1.3	-1.0	-1.7	-1.8	-0.9	-1.9
0178dib	dibromomethane	-2.1	-2.4	-1.9	-1.7	-2.3	-2.2	-2.3
0179tri	bromoform	-2.0	-1.9	-2.2	-0.3	-2.0	-2.1	-1.9
0180bro	bromoethane	-0.7	-0.9	-0.7	-1.6	-0.7	-1.2	-1.9
0182bro	1-bromopropane	-0.6	-0.4	-0.4	-1.3	-0.7	-1.1	-2.0
0183bro	2-bromopropane	-0.5	-0.5	-0.4	-1.6	-0.7	-1.0	-2.0
0184bro	1-bromobutane	-0.4	-0.2	-0.3	-1.1	-0.8	-1.0	-2.0
0185bro	1-bromopentane	-0.1	-0.0	-0.2	-0.9	-0.1	-0.8	-2.0
0186bro	bromobenzene	-1.5	-1.5	-1.7	-0.8	-1.3	-1.4	-1.9
0187dib	p-dibromobenzene	-2.3	-0.9	-2.0	-0.3	-1.1	-1.9	-1.9
0197bro	bromotrifluoromethane	1.8	1.6	1.4	2.1	3.0	2.2	-0.6
0198chl	chlorofluoromethane	-0.8	-2.7	-1.3	-1.5	-1.0	-1.4	-2.3
0199chl	chlorodifluoromethane	-0.5	-2.3	-0.5	-0.9	0.0	-0.3	-1.9
0200tet	tetrafluoromethane	3.2	1.9	2.6	2.0	2.3	3.2	-0.4
0201bro	1-bromo-1-chloro-2,2,2-trif	-0.1	-0.9	-0.0	-0.0	0.1	-0.1	-2.0
0202bro	1-bromo-2-chloroethane	-1.9	-2.3	-1.5	-1.9	-1.5	-2.5	-2.4
0203bro	1-bromo-1,2,2,2-tetrafluoroeth	0.5	-0.5	0.4	0.6	1.2	0.2	-2.0
0204tet	tetrachloroethene	0.1	0.0	-0.1	-0.3	0.2	1.9	-0.8
0205chl	1-chloro-2,2,2-trifluoroethane	0.1	-1.2	0.1	-0.9	-0.2	-1.1	-2.5
0206tri	1,1,2-trichloro-1,2,2-trifluoroe	1.8	1.6	1.4	0.9	1.3	2.9	-0.7
0207tri	2,2,2-trifluoroethanol	-4.3	-4.8	-5.1	-5.4	-4.1	-5.3	-4.9
0209chl	1-chloro-2,2,2-trifluoroethy	0.1	-2.9	-0.7	-1.1	-0.3	-0.7	-3.0
0211tri	1,1,1-trifluoropropan-2-ol	-4.2	-2.0	-2.7	-3.5	-2.8	-3.9	-3.6
0212hex	1,1,1,3,3,3-hexafluoropropan-2-	-3.8	-2.4	-1.9	-3.5	-1.1	-2.5	-3.4
0213bis	bis(2-chloroethyl)sulfide	-3.9	-3.8	-2.2	-1.8	-4.0	-4.2	-3.9
0214tri	2,2,2-trifluorethylvinylether	-0.1	-1.0	-0.5	-0.7	-0.7	-0.5	-2.9
0215pbr	p-bromophenol	-7.1	-5.5	-6.9	-6.1	-6.0	-6.0	-4.3
0216amm	ammonia	-4.3	-4.5	-5.2	-6.8	-5.9	-3.6	-3.4
0217wat	water	-6.3	-7.5	-8.1	-9.1	-7.6	-8.0	-4.7
0218pho	phosphine	0.6	0.6	0.6	2.0	0.7	0.9	-0.6
0219hyd	hydrogensulfide	-0.7	-2.4	-2.0	-1.4	-1.0	-1.3	-1.9
0220tri	trimethylphosphate	-8.7	-10.2	-10.2	-8.3	-7.2	-5.3	-6.7
0221tri	triethylphosphate	-7.8	-7.5	-8.2	-8.2	-7.2	-6.2	-7.0
0222tri	tripropylphosphate	-6.1	-5.8	-6.9	-6.8	-6.9	-6.0	-7.0
0223die	diethyldisulfide	-1.6	-1.1	-0.4	-0.2	-0.4	-0.9	-2.2
0225pipa	piperidine	-5.1	-2.3	-2.9	-2.1	-1.6	-3.3	-1.8
0227Nme	N-methylmorpholine	-6.3	-4.7	-4.5	-2.3	-2.5	-5.4	-2.7
0228met	methylamine	-4.6	-3.6	-4.2	-4.7	-4.5	-3.6	-2.7
0229hyd	hydrazine	-6.3	-8.6	-10.0	-9.2	-9.4	-5.3	-4.8
0230eth	2-ethylpyrazine	-5.5	-6.8	-5.2	-4.9	-4.3	-5.4	-3.4
0233ethb	acetamide	-9.7	-10.6	-10.5	-9.8	-10.4	-9.0	-6.9
0234ENmb	E-N-methylacetamide	-10.0	-9.2	-8.6	-7.8	-8.8	-8.6	-6.6
0235ZNmb	Z-N-methylacetamide	-10.0	-9.3	-9.2	-8.6	-8.5	-8.6	-6.5
0236oct	1-octanol	-4.1	-2.9	-3.7	-3.5	-3.0	-3.4	-3.3

0237oct	octanal	-2.3	-4.0	-2.5	-2.3	-2.4	-2.2	-3.7
0238met	methyloctanoate	-2.0	-2.3	-2.5	-2.4	-3.1	-1.9	-3.7
0239oct	2-octanone	-2.9	-3.3	-2.4	-2.9	-3.2	-3.2	-4.1
0240met	methylbenzoate	-3.9	-3.8	-3.7	-3.4	-3.6	-2.7	-3.8
0242dii	isopropylether	-0.5	-1.0	-1.0	-1.1	-1.5	-1.0	-1.9
0244tet	tetrahydropyran	-3.1	-2.0	-2.0	-0.8	-1.0	-2.0	-1.9
0245thi	thiophene	-1.4	-1.7	-1.3	-0.9	-2.2	-0.6	-1.8
0246eth	ethylphenylether	-2.2	-2.6	-2.4	-1.7	-1.9	-1.6	-2.6
0400hyd	hydrogen	2.3	0.7	0.5	0.4	0.6	1.6	-0.1
0401amia	1,1-dimethyl-3-phenylurea	-9.6	-8.0	-9.4	-7.3	-8.3	-8.5	-7.0
0402adn	9-methyladenine	-13.6	-15.5	-14.4	-13.5	-15.3	-13.6	-7.6
0403thi	1-methylthymine	-10.4	-12.0	-11.4	-10.5	-13.1	-11.2	-8.8
0405hex	hexafluoroethane	3.9	3.5	3.5	3.9	3.8	4.2	-0.4
0406oct	octafluoropropane	4.3	4.4	4.3	4.9	4.3	5.1	-0.5
0407tet	1,1,1,2-tetrachloroethane	-1.1	-2.3	-1.5	-2.1	-2.1	-1.6	-2.1
0408hex	hexachloroethane	-1.4	-0.0	-0.5	-1.0	-4.1	1.3	-1.0
0409clb	2-chlorobutane	0.1	-0.6	-0.1	-0.7	-0.1	-0.5	-1.8
0410clp	1-chloropentane	0.1	-0.4	-0.1	-0.2	0.1	-0.6	-2.0
0411chp	2-chloropentane	0.1	-0.1	0.2	-0.3	0.2	-0.3	-1.8
0412clt	chlorotoluene	-1.9	-3.3	-2.4	-1.8	-2.7	-2.6	-3.1
0413clt	o-chlorotoluene	-1.1	-0.6	-0.8	-0.5	-0.8	-0.4	-1.7
0414dcl	2,2'-dichlorobiphenyl	-2.7	-2.2	-2.0	-1.2	-2.2	-1.8	-3.1
0415dcl	2,3-dichlorobiphenyl	-2.5	-2.0	-1.6	-1.2	-1.9	-1.5	-2.9
0416dcl	2,2',3'-trichlorobiphenyl	-2.0	-2.0	-1.8	-1.1	-2.1	-1.7	-3.2
0417brp	3-bromopropene	-0.9	-1.7	-1.1	-1.9	-2.5	-1.3	-2.3
0418bri	1-bromo-isobutane	-0.0	-0.1	-0.1	-1.1	-1.0	-0.7	-1.9
0419brt	bromotoluene	-2.4	-3.0	-2.5	-2.5	-3.3	-2.8	-3.1
0420pbr	p-bromotoluene	-1.4	-0.8	-1.5	-0.7	-1.0	-1.1	-1.9
0421dfl	difluorodichloromethane	1.7	1.0	1.2	0.4	1.5	2.3	-0.5
0422ftc	fluorotrichloromethane	0.8	0.5	0.4	-0.3	0.4	1.7	-0.6
0423brt	bromotrichloromethane	-0.9	0.0	-0.8	-0.1	-1.4	0.4	-0.8
0424clp	chloropentaflouroethane	2.9	2.9	2.9	2.9	3.1	3.9	-0.5
0425dbr	3,5-dibromo-4-hydroxybenzoni	-9.0	-7.7	-9.0	-8.7	-7.9	-4.6	-6.2
0426dcl	2,6-dichlorobenzonitrile	-5.2	-5.2	-4.3	-5.0	-6.0	-3.2	-5.3
0427dcl	2,6-dichlorothiobenzamide	-10.8	-10.4	-10.2	-9.4	-8.0	-8.6	-7.4
0428ami	4-amino-3,5,6-trichloropyrid	-11.9	-11.4	-13.4	-14.1	-12.5	-10.6	-8.0
0433pho	2,2-dichloroethenyldimethylp	-6.6	-8.0	-8.1	-7.5	-6.0	-3.5	-5.8
0437pho	methyl3-methyl-4-thiomethoxy	-6.9	-11.0	-11.0	-10.1	-8.0	-7.3	-7.8
0438pho	diethyl2,4-dichloropheny	-3.9	-3.7	-4.0	-3.9	-2.8	-2.6	-4.7
0440pho	dimethyl5-(4-chloro)bicyclo	-7.3	-7.3	-7.6	-6.8	-4.9	-4.5	-5.8
0441pho	dimethyl4-nitrophenylthiop	-7.6	-8.0	-7.7	-7.2	-7.1	-4.1	-7.5
0442pho	O-ethyl-O'-4-bromo-2-c	-4.1	-6.2	-7.1	-6.2	-6.2	-6.8	-7.3
0444pho	dimethyl2,4,5-trichlorophe	-5.1	-4.8	-5.1	-4.8	-2.9	-2.1	-4.9
0445pho	dimethyl4-bromo-2,5-dic	-5.7	-4.8	-5.6	-4.6	-2.6	-2.5	-4.9
0447pho	diethyl4-nitrophenylthiop	-6.3	-6.4	-6.2	-6.3	-6.4	-4.4	-7.2
0449pho	ethyl4-cyanophenylphenylt	-5.1	-8.7	-7.6	-9.0	-9.6	-5.7	-8.1
0471dim	3,4-dimethylpyridine	-5.2	-4.7	-4.2	-3.9	-4.8	-4.3	-3.6
0506nit	nitromethane	-4.0	-7.4	-6.0	-5.2	-5.3	-3.7	-5.2
0571dim	3,5-dimethylpyridine	-4.8	-4.3	-3.8	-3.7	-4.4	-3.8	-3.5
0574eth	4-ethylpyridine	-4.7	-5.1	-4.2	-3.7	-4.3	-4.1	-3.5
0939tet	tetramethylsilane	3.0	0.9	1.3	-0.4	0.6	3.8	-0.6
c000	water dimer	-11.2	-16.7	-15.3	-16.1	-14.0	-13.4	-7.9
n005	methylhydrazine	-5.3	-7.3	-8.9	-7.2	-7.2	-5.1	-4.2
n006	1,1-dimethylhydrazine	-4.5	-5.6	-6.8	-4.8	-5.8	-4.7	-3.4
n007	urea	-13.8	-14.6	-15.7	-14.2	-14.4	-12.1	-8.5
n008	benzamide	-10.9	-10.0	-10.2	-9.5	-9.4	-8.9	-6.8
n009	2-methylaniline	-5.6	-4.6	-6.1	-5.6	-6.1	-4.3	-3.9
n010	3-methylaniline	-5.7	-5.1	-6.5	-6.1	-6.3	-4.3	-4.0
n011	4-methylaniline	-5.5	-5.1	-6.5	-6.0	-4.9	-4.2	-4.0
n013	N-ethylaniline	-4.6	-4.4	-4.9	-4.0	-4.0	-3.5	-3.4
n014	N,N-dimethylaniline	-3.6	-4.2	-4.0	-2.4	-1.9	-2.3	-2.8
n015	3-aminoaniline	-9.9	-9.4	-12.3	-11.5	-10.7	-8.7	-6.5
n016	1,2-ethanediamine	-9.7	-6.8	-8.3	-9.4	-8.7	-9.1	-5.3
n017	hydrogen peroxide	-8.6	-8.9	-10.4	-10.2	-6.5	-8.9	-4.7
n018	methyl peroxide	-5.3	-5.8	-7.0	-6.1	-4.3	-5.5	-3.7
n019	ethyl peroxide	-5.3	-5.2	-6.6	-5.8	-4.4	-5.6	-3.7
n191	uracil	-16.5	-16.7	-15.7	-14.0	-15.7	-13.6	-10.2
n200	5-fluorouracil	-16.9	-15.8	-14.7	-13.8	-15.2	-13.5	-10.6
n201	5-trifluoromethyluracil	-15.4	-14.5	-13.7	-13.6	-13.5	-13.0	-11.1
n202	5-chlorouracil	-17.7	-16.5	-15.3	-14.5	-15.4	-13.6	-10.4
n203	5-bromouracil	-18.1	-16.3	-15.8	-14.1	-14.6	-13.6	-10.5
test0001	1,3-diacetyloxypropan-2-ylacetat	-8.8	-9.8	-10.3	-9.9	-12.4	-10.0	-8.3
test0004	m-bis(trifluoromethyl)benzene	1.1	4.1	3.3	2.6	1.5	0.9	-2.6
test0005	N,N-dimethyl-p-methoxybenzami	-11.0	-8.1	-8.1	-6.4	-7.5	-7.3	-7.0
test0006	N,N,4-trimethylbenzamide	-9.8	-6.2	-6.1	-5.4	-6.6	-6.2	-5.9
test0007	bis(2-chloroethyl)ether	-4.2	-3.9	-3.1	-1.7	-2.3	-3.8	-3.3
test0008	1,1-diacetoxyethane	-5.0	-6.2	-6.1	-6.4	-8.0	-5.6	-5.8
test0009	1,1-diethoxyethane	-3.3	-2.3	-2.5	-1.3	-2.4	-1.9	-2.4
test0011	diethylpropanedioate	-6.0	-6.8	-6.4	-6.6	-7.8	-6.0	-6.1
test0012	dimethoxymethane	-2.9	-3.8	-3.7	-1.4	-2.5	-1.8	-2.5
test0013	ethyleneglycoldiacetate	-6.3	-6.5	-7.2	-6.2	-7.1	-6.0	-5.3

test0014	1,2-diethoxyethane	-3.5	-3.6	-3.7	-0.8	-1.1	-2.1	-2.6
test0016	phenylformate	-3.8	-6.2	-4.3	-3.2	-5.2	-2.8	-4.1
test0017	imidazole	-9.8	-12.4	-11.2	-10.8	-9.4	-9.0	-6.7
test1001	nitroglycol	-5.7	-5.1	-4.8	-4.3	-4.1	-1.2	-6.3
test1002	1,2-dinitroxypropane	-5.0	-5.0	-4.9	-4.7	-4.3	-1.7	-6.7
test1003	butylnitrate	-2.1	-1.6	-1.8	-1.4	-1.5	-0.1	-3.8
test1004	2-butylnitrate	-1.8	-1.2	-1.6	-1.6	-1.3	0.0	-3.5
test1005	isobutylnitrate	-1.9	-1.5	-1.6	-1.5	-1.8	0.1	-3.7
test1006	ethyleneglycolmononitrate	-8.2	-7.3	-7.2	-6.5	-6.9	-4.9	-5.7
test1007	2-chloro-N-(2,6-diethylphe	-8.2	-6.5	-5.8	-4.9	-5.5	-5.2	-5.5
test1008	2-methyl-2-(methylthio)propa	-9.8	-8.3	-7.8	-6.5	-8.3	-6.8	-6.8
test1009	2-(ethylamino)-4-isopropylamin	-7.7	-8.9	-10.0	-8.7	-7.7	-8.5	-5.8
test1010	O,O-dimethylS-[(4-oxo-1,2	-10.0	-10.3	-9.6	-6.6	-11.6	-11.6	-9.7
test1011	N-butyl-N-ethyl-2,6-dinitro	-3.5	-1.2	-0.5	-2.4	-2.7	-0.8	-6.3
test1012	bensulfuron	-17.2	-27.9	-28.5	-26.9	-25.3	-26.6	-19.5
test1013	5-bromo-3-sec-butyl-6-methy	-9.7	-8.8	-9.4	-10.1	-10.5	-9.6	-8.5
test1014	3a,4,7,7a-tetrahydro-2-[(t	-9.0	-7.5	-6.7	-7.4	-7.4	-7.6	-7.2
test1015	1-naphthylmethylcarbamate(car	-9.5	-8.7	-8.5	-8.6	-8.6	-8.8	-7.6
test1016	2,3-dihydro-2,2-dimethyl-7-be	-9.6	-8.7	-9.1	-9.1	-8.3	-9.5	-8.8
test1017	S-4-chlorophenylthiometh	-6.5	-5.2	-5.5	-3.6	-2.7	-2.7	-4.8
test1018	octachloro-4,7-methanohydroinda	-3.4	-2.2	-1.9	-2.9	-3.7	-3.9	-4.4
test1019	phosphoricacid[(E)-2-chlor	-7.1	-6.5	-7.1	-6.9	-7.1	-5.6	-7.1
test1020	ethyl2-(4-chloro-6-metho	-14.0	-17.2	-17.8	-19.0	-17.2	-18.4	-13.8
test1021	trichloro(nitro)methane(chloro	-1.5	-1.9	-1.5	-2.6	-1.9	1.8	-2.4
test1022	O,O-diethylO-3,5,6-tric	-5.0	-5.0	-5.1	-5.0	-2.5	-1.8	-4.8
test1023	S-(RS)-2-chloro-1-phth	-5.7	-10.7	-8.9	-8.4	-8.7	-9.1	-8.7
test1024	diethoxy-[(2-isopropyl-6-	-6.5	-6.1	-6.7	-8.0	-7.5	-7.0	-6.7
test1025	3,6-dichloro-2-methoxybenzoica	-9.9	-7.1	-8.3	-7.4	-6.2	-5.4	-5.1
test1027	N1,N1-diethyl-2,6-dinitro-4	-5.7	-3.1	-4.4	-5.0	-6.6	-3.7	-7.3
test1028	(RS)-2-sec-butyl-4,6-dinitrop	-6.2	-9.9	-9.4	-10.7	-10.1	-8.4	-10.1
test1029	6,7,8,9,10,10-hexachloro-1,5	-4.2	-10.1	-9.4	-13.1	-4.5	-8.8	-6.8
test1030	(1R,4S,4aS,5S,6S,7R,8R,8aR)-1	-5.5	-5.1	-3.7	-3.6	-3.8	-4.4	-4.3
test1031	O,O,O',O'-tetraethylS,S'-met	-6.1	-7.9	-8.5	-7.2	-6.8	-7.2	-8.2
test1033	1,4,5,6,7,8,8-heptachloro-3a,4,	-2.6	-1.8	-1.8	-1.9	-2.6	-2.0	-3.2
test1034	3,5,5-trimethyl-2-cyclohexen-1-o	-5.2	-4.2	-3.7	-4.3	-5.2	-5.2	-5.3
test1035	1,2,3,4,5,6-hexachlorocyclohexan	-5.4	-7.2	-3.8	-5.2	-5.3	-6.4	-4.9
test1036	2-(dimethoxyphosphinothioyl	-8.2	-9.8	-11.2	-8.5	-7.9	-6.5	-8.0
test1037	N-methylcarbamicacid[1-(meth	-10.7	-9.1	-10.7	-9.0	-8.5	-8.1	-7.6
test1039	methyl2-(4-methoxy-6-methyl	-15.5	-19.4	-19.6	-21.0	-21.2	-22.0	-15.7
test1040	4-mesyl-2,6-dinitro-N,N-dip	-8.0	-12.7	-9.8	-13.4	-11.8	-10.4	-11.5
test1041	nitroxyacetone	-6.0	-6.1	-4.8	-5.3	-6.1	-3.9	-5.9
test1043	O,O-diethyl-O-4-nitro-phe	-6.7	-6.7	-6.7	-7.0	-7.0	-5.0	-7.8
test1044	S-propylbutyl(ethyl)thiocar	-3.6	-2.6	-3.1	-2.4	-3.0	-3.1	-4.2
test1045	O,O-diethylS-ethylthiomethyl	-4.4	-5.2	-5.1	-4.3	-4.0	-4.5	-5.7
test1046	N-cyclopropylmethyl-2,6-din	-2.5	-1.5	-0.8	-2.7	-3.7	-2.2	-6.6
test1047	N2,N4-diisopropyl-6-methylthi	-8.4	-7.8	-9.3	-8.4	-8.0	-8.3	-5.8
test1048	N-(3,4-dichlorophenyl)propan	-7.8	-7.4	-8.1	-7.2	-7.0	-7.0	-6.3
test1049	5-amino-4-chloro-2-phenyl-3	-16.4	-12.7	-12.1	-11.3	-12.8	-11.7	-9.4
test1050	6-chloro-N,N'-diethyl-1,3,5-t	-10.2	-8.6	-10.2	-9.7	-12.0	-11.6	-6.3
test1051	methyl2-(4,6-dimethylpyrimi	-20.3	-20.3	-20.2	-21.5	-19.4	-21.2	-15.7
test1052	3-t-butyl-5-chloro-6-methyl	-11.1	-8.1	-8.2	-9.9	-9.9	-8.8	-7.8
test1053	N2-tert-butyl-N4-ethyl-6-meth	-6.7	-7.9	-9.4	-8.1	-7.6	-7.9	-5.6
test1054	3-(4-methoxy-6-methyl-1,3,5	-16.2	-20.9	-21.5	-23.2	-22.2	-23.2	-17.0
test1055	dimethyl(RS)-2,2,2-trichloro	-12.7	-12.4	-12.7	-11.9	-10.6	-8.3	-7.7
test1056	a,a,a-trifluoro-2,6-dinitro	-3.3	-1.0	-0.6	-2.5	-3.0	-1.4	-6.5
test1057	S-propyldipropyl(thiocarbam	-4.1	-2.2	-2.6	-2.2	-3.0	-3.3	-4.1
test1058	4-amino-4'-nitroazobenzene	-11.2	-11.3	-11.2	-10.0	-10.0	-8.9	-8.5
test1059	1-amino-4-anilinoanthraquinon	-7.4	-8.2	-8.6	-7.8	-10.8	-8.4	-6.8
test1060	1,4,5,8-tetraminoanthraquinon	-8.9	-12.7	-18.0	-15.0	-15.7	-13.0	-9.2
test1061	1-amino-anthraquinone	-8.0	-7.1	-7.2	-7.4	-10.7	-7.5	-6.2
test1063	(2-dimethylamino-5,6-dimethyl	-9.4	-9.1	-9.9	-7.8	-7.1	-7.7	-7.0
test2001	acetylsalicylicacid	-9.9	-9.8	-10.2	-9.1	-9.4	-7.6	-6.6
test2003	butylparaben	-8.7	-7.0	-8.2	-8.5	-8.7	-7.5	-6.5
test2004	caffeine	-12.6	-12.0	-10.7	-11.4	-13.0	-11.6	-8.4
test2006	6-chlorouracil	-15.8	-13.3	-13.3	-12.7	-13.5	-11.1	-8.5
test2007	cyanuricacid	-18.0	-18.7	-18.0	-17.5	-18.4	-14.4	-10.3
test2010	diflunisal	-9.4	-11.4	-13.0	-13.7	-11.9	-12.1	-9.3
test2011	ethylparaben	-9.2	-7.7	-8.7	-9.0	-9.3	-7.7	-6.4
test2013	flurbiprofen(racemic)	-8.4	-6.9	-7.3	-7.4	-8.3	-6.8	-6.2
test2015	hexachlorobenzene	-2.3	-1.0	0.3	-0.8	0.2	1.4	-1.6
test2017	ibuprofen(racemic)	-7.0	-6.2	-6.9	-6.6	-7.2	-5.1	-5.1
test2018	5-iodouracil	-18.7	-16.1	-16.1	-14.6	-15.4	-14.8	-10.4
test2019	ketoprofen(racemic)	-10.7	-10.4	-9.8	-10.5	-10.7	-9.7	-7.7
test2020	methylparaben	-9.5	-8.3	-9.3	-9.0	-8.2	-7.4	-6.3
test2021	naproxen	-10.2	-9.3	-10.0	-8.6	-9.5	-7.8	-6.7
test2022	4-nitroaniline	-9.4	-9.7	-10.3	-9.2	-9.3	-8.1	-8.2
test2023	octafluorocyclobutane	3.4	4.9	4.5	4.8	2.6	3.3	-1.4
test2024	pentachloronitrobenzene	-5.2	-3.9	-1.4	-3.0	-1.0	2.0	-3.4
test2025	phthalimide	-9.6	-10.5	-9.0	-8.9	-11.0	-8.3	-6.8
test2026	propylparaben	-9.4	-7.2	-8.4	-8.6	-9.4	-7.6	-6.4
test2027	sulfolane	-8.6	-11.8	-9.4	-11.0	-8.9	-11.4	-8.0

test2029	trimethylorthotrifluoroacetate	-0.8	-0.5	-1.8	-0.2	-0.0	0.2	-3.0
test3001	paracetamol	-14.8	-12.4	-13.9	-12.8	-13.0	-12.1	-8.6
test3002	N-(3-hydroxyphenyl)acetamide	-13.9	-12.4	-13.8	-13.0	-12.3	-11.8	-8.6
test3003	fenbufen	-12.7	-14.8	-14.0	-15.3	-14.7	-14.3	-10.7
test3004	N-(2-hydroxyphenyl)acetamide	-11.6	-10.8	-11.9	-11.2	-11.5	-10.0	-7.4
test3005	phenacetin	-10.9	-9.3	-10.0	-8.2	-9.3	-8.5	-7.3
test3007	2-methoxybenzoicacid	-10.3	-8.9	-9.7	-9.0	-9.2	-7.2	-6.1
test3014	4-methoxybenzoicacid	-9.2	-8.4	-9.2	-8.1	-8.6	-6.4	-5.7
test3015	3-methoxybenzoicacid	-8.9	-8.6	-9.1	-8.1	-8.2	-6.3	-5.6
test3019	tolfenamicacid	-6.7	-5.8	-6.6	-6.2	-6.9	-4.9	-4.6
test3020	diclofenacacid	-6.3	-9.9	-10.6	-9.5	-10.7	-10.4	-9.2
test3021	flufenamicacid	-5.7	-6.5	-8.5	-8.2	-9.2	-9.9	-9.8
test4001	iodobenzene	-1.7	-1.7	-2.1	-1.1	-1.1	-1.7	-1.9
test4002	diiodomethane	-2.5	-2.2	-2.2	-2.2	-2.4	-3.5	-2.2
test4003	iodomethane	-0.9	-1.2	-1.0	-1.1	-1.5	-0.9	-1.7
test4004	iodoethane	-0.7	-0.8	-0.7	-0.8	-0.6	-1.1	-1.8
test4006	1-iodopropane	-0.6	-0.4	-0.5	-0.5	-0.6	-1.0	-1.8
test4007	1-iodobutane	-0.2	-0.3	-0.4	-0.3	-0.5	-0.8	-1.8
test4008	1-iodopentane	-0.1	0.0	-0.2	-0.1	-0.4	-0.7	-1.9
test4009	2-iodopropane	-0.5	-0.5	-0.5	-0.6	-0.4	-0.9	-1.8

Table S5. Solvation free energies in *toluene* for the 50-molecule dataset in kcal·mol^{-1}. The codes of the molecules correspond to those in the Minnesota Solvation Database.[1]

Code	Name	exper.	ESE-CM5	SMD	PCM
0008noc	n-octane	-5.4	-5.8	-5.2	-0.1
0036tol	toluene	-5.1	-6.2	-5.2	-0.7
0044met	methanol	-2.2	-3.0	-1.7	-1.5
0045eth	ethanol	-3.3	-3.8	-2.8	-1.4
0047pro	1-propanol	-3.7	-4.3	-3.5	-1.4
0049but	1-butanol	-4.3	-4.9	-4.2	-1.4
0052pen	1-pentanol	-5.2	-5.1	-4.9	-1.5
0053phe	phenol	-6.9	-7.0	-5.9	-1.7
0054hex	1-hexanol	-6.1	-5.6	-5.5	-1.5
0055ocr	o-cresol	-7.4	-7.6	-6.1	-1.6
0057pcr	p-cresol	-7.6	-7.5	-6.2	-1.7
0058hep	1-heptanol	-6.8	-6.2	-6.1	-1.5
0062dio	1,4-dioxane	-4.9	-4.1	-3.9	-1.5
0075pro	acetone	-3.6	-3.9	-4.3	-1.9
0076but	2-butanone	-4.3	-4.4	-4.8	-1.8
0078pen	2-pentanone	-5.0	-4.9	-5.4	-1.8
0080hex	2-hexanone	-5.6	-5.5	-6.0	-1.8
0081dim	3,3-dimethylbutanone	-5.0	-5.1	-5.1	-1.7
0082hep	2-heptanone	-6.3	-6.0	-6.6	-1.8
0086eth	acetic acid	-4.0	-4.0	-3.9	-2.2
0087pro	propanoic acid	-4.6	-4.6	-4.5	-2.0
0088but	butanoic acid	-5.2	-5.0	-5.1	-2.1
0089pen	pentanoic acid	-5.9	-5.6	-5.7	-2.1
0090hex	hexanoic acid	-7.0	-6.1	-6.4	-2.1
0093met	methyl acetate	-3.8	-4.1	-3.3	-1.8
0094met	methyl propanoate	-4.6	-4.8	-3.8	-1.6
0095eth	ethyl acetate	-4.4	-4.6	-4.4	-1.8
0097pro	propyl acetate	-5.0	-5.1	-5.1	-1.8
0098met	methyl pentanoate	-5.7	-5.6	-5.1	-1.7
0099but	butyl acetate	-5.6	-5.7	-5.8	-1.8
0100met	methyl hexanoate	-6.4	-6.1	-5.7	-1.7
0101pen	pentyl acetate	-6.4	-6.2	-6.4	-1.8
0103eth	ethylamine	-2.7	-3.0	-2.4	-1.2
0104dim	dimethylamine	-2.7	-3.5	-2.0	-0.9
0106pro	propylamine	-3.5	-3.5	-3.1	-1.2
0107tri	trimethylamine	-2.7	-4.0	-2.5	-0.6
0110but	butylamine	-4.3	-4.1	-3.7	-1.3
0111die	diethylamine	-3.8	-3.9	-3.4	-0.8
0115dip	dipropylamine	-5.2	-5.2	-4.5	-0.9
0116pyr	pyridine	-5.1	-4.7	-4.8	-1.4
0118ani	aniline	-6.7	-7.0	-5.7	-1.8
0131nit	1-nitropropane	-5.2	-5.2	-5.2	-2.4
0215pbr	p-bromophenol	-8.7	-7.6	-7.4	-2.0
0216amm	ammonia	-2.4	-1.0	-1.0	-1.6
0217wat	water	-1.7	-2.3	-2.7	-2.2
0228met	methylamine	-2.6	-2.6	-1.6	-1.2
0240met	methyl benzoate	-8.0	-6.9	-6.1	-1.8
0506nit	nitromethane	-4.3	-4.6	-3.9	-2.5
n011	4-methylaniline	-7.4	-7.4	-5.9	-1.7
n017	hydrogen peroxide	-3.1	-3.8	-3.6	-2.2

[1] A. V. Marenich, C. P. Kelly, J. D. Thompson, G. D. Hawkins, C. C. Chambers, D. J. Giesen, P. Winget, C. J. Cramer, and D. G. Truhlar, Minnesota Solvation Database – version 2012, University of Minnesota, November 26, 2012. https://comp.chem.umn.edu/mnsol/MNSol-v2012_Manual.pdf retrieved on 28/05/2019.