Supporting Information

Generalized Born Solvation Model SM12

Aleksandr V. Marenich, Christopher J. Cramer, and Donald G. Truhlar

Department of Chemistry, Chemical Theory Center, and Supercomputing Institute,

University of Minnesota, 207 Pleasant Street S.E.,

Minneapolis, MN 55455-0431

Prepared for *The Journal of Chemical Theory and Computation*

Revised on November 27, 2012

Number of pages: 59

Contents:

Table S1. Reference Solvation Free Energies (kcal/mol) for 274 Neutral Solutes in Water

solute	free energy of solvation
1,1,1,2-tetrachloroethane	-1.15
1,1,1,3,3,3-hexafluoropropan-2-ol	-3.77
1,1,1-trichloroethane	-0.25
1,1,1-trifluoropropan-2-ol	-4.16
1,1,2-trichloro-1,2,2-trifluoroethane	1.77
1,1,2-trichloroethane	-1.95
1,1-difluoroethane	-0.11
1,1-dimethyl-3-phenylurea	-9.63
1,1-dimethylhydrazine	-4.48
1,2-dichlorobenzene	-1.36
1,2-dichloroethene	-0.76
1,2-dichloroethene	-1.17
1,2-dimethoxyethane	-4.84
1,2-ethanediamine	-9.72
1,2-ethanediol	-9.30
1,4-dichlorobenzene	-1.01
1,4-dioxane	-5.05
1-bromo-1,2,2,2-tetrafluoroethane	0.52
1-bromo-1-chloro-2,2,2-trifluoroethane	-0.13
1-bromo-2-chloroethane	-1.95
1-bromobutane	-0.41
1-bromo-isobutane	-0.03
1-bromopentane	-0.08
1-bromopropane	-0.56
1-butanol	-4.72
1-butene	1.38
1-butyne	-0.16
1-chloro-2,2,2-trifluoroethane	0.06
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	0.11
1-chloropentane	0.07
1-chloropropane	-0.27
1-heptanol	-4.24
1-hexanol	-4.36
1-hexene	1.68
1-hexyne	0.29
1-methylthymine	-10.40
1-nitrobutane	-3.08
1-nitropropane	-3.34
1-octanol	-4.09
1-pentanol	-4.47
1-pentene	1.66
1-pentyne	0.01
1-propanethiol	-1.05
1-propanol	-4.83
2,2,2-trifluorethyl vinyl ether	-0.12
2,2,2-trifluoroethanol	-4.31
2,2',3'-trichlorobiphenyl	-1.99
2,2,4-trimethylpentane	2.85
2,2'-dichlorobiphenyl	-2.73
2,2-dichloroethenyl dimethyl phosphate	-6.61
2,2-dimethylpropane	2.50
2,3-dichlorobiphenyl	-2.45
2,4-dimethylpentane	2.88
2,4-dimethylpyridine	-4.86
2,5-dimethylpyridine	-4.72
2,6-dichlorobenzonitrile	-5.22
2,6-dichlorothiobenzamide	-10.81
2,6-dimethylpyridine	-4.60
2-bromopropane	-0.48
2-butanone	-3.64
2-chlorobutane	0.07
2-chloropentane	0.07
2-chloropropane	-0.25
2-ethylpyrazine	-5.51
2-heptanone	-3.04

2-hexanone	-3.29
2-methoxyethanamine	-6.55
2-methoxyethanol	-6.77
2-methyl-1-nitrobenzene	-3.59
2-methylaniline	-5.56
2-methylpentane	2.52
2-methylpropane	2.32
2-methylpropene	1.16
2-methylpyrazine	-5.57
2-methylpyridine	-4.63
2-nitropropane	-3.14
2-octanone	-2.88
2-pentanone	-3.53
2-pentene	1.34
3,3-dimethylbutanone	-2.89
3,4-dimethylpyridine	-5.22
3,5-dibromo-4-hydroxybenzonitrile	-9.00
3,5-dimethylpyridine	-4.84
3,aminoaniline	-9.92
3-bromopropene	-0.86
3-chloropropene	-0.57
3-methylaniline	-5.67
3-methylpyridine	-4.77
3-pentanone	-3.41
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	-11.96
4-ethylpyridine	-4.74
4-heptanone	-2.93
4-methylaniline	-5.55
4-methylpyridine	-4.94
5-nonanone	-2.67
9-methyladenine	-13.60
acetaldehyde	-3.50
acetamide	-9.71
acetic acid	-6.70
acetone	-3.85
acetonitrile	-3.89
acetophenone	-4.58
allyl alcohol	-5.08
ammonia	-4.29
aniline	-5.49
anisole	-2.45
anthracene	-4.23
azetidine	-5.56
benzaldehyde	-4.02
benzamide	-10.90
benzene	-0.87
benzonitrile	-4.10
bis(2-chloroethyl)sulfide	-3.92
bromobenzene	-1.46
bromoethane	-0.70
bromomethane	-0.82
bromotoluene	-2.37
bromotrichloromethane	-0.93
bromotrifluoromethane	1.79
butanal	-3.18
butanoic acid	-6.36
butanonitrile	-3.64
butenyne	0.04
butyl acetate	-2.55
butylamine	-4.29
chlorobenzene	-1.12
chlorodifluoromethane	-0.50
chloroethane	-0.63
chloroethene	-0.59
chlorofluoromethane	-0.77
chloroform	-1.07
chloromethane	-0.56
chloropentaflouroethane	2.86
chlorotoluene	-1.92
cis-1,2-dimethylcyclohexane	1.58

cyclohexane	1.23
cyclopentane	1.20
cyclopentanol	-5.49
cyclopentanone	-4.68
cyclopentene	0.56
cyclopropane	0.75
dibromomethane	-2.11
dichloromethane	-1.36
diethyl 2,4-dichlorophenyl thiophosphate	-3.86
diethyl 4-nitrophenyl thiophosphonate	-6.27
diethyl disulfide	-1.63
diethyl ether	-1.76
diethyl sulfide	-1.43
diethylamine	-4.07
difluorodichloromethane	1.69
dimethyl 2,4,5-trichlorophenyl thiophosphate	-5.06
dimethyl 4-bromo-2,5-dichlorophenyl thiophosphate	-5.70
dimethyl 4-nitrophenyl thiophosphate	-7.62
dimethyl 5-(4-chloro)bicyclo[3.2.0]heptyl phosphate	-7.28
dimethyl disulfide	-1.83
dimethyl ether	-1.92
dimethyl sulfide	-1.54
dimethylamine	-4.29
dipropyl sulfide	-1.27
dipropylamine	-3.66
ethane	1.83
ethanethiol	-1.30
ethanol	-5.01
ethene	1.27
ethyl 4-cyanophenyl phenylthiophosphonate	-5.10
ethyl acetate	-3.10
ethyl formate	-2.65
ethyl peroxide	-5.32
ethyl phenyl ether	-2.22
ethylamine	-4.50
ethylbenzene	-0.80
ethyne	-0.01
fluorobenzene	-0.78
fluoromethane	-0.22
fluorotrichloromethane	0.82
hexachloroethane	-1.40
hexafluoroethane	3.94
hexanoic acid	-6.21
hydrazine	-6.26
hydrogen	2.33
hydrogen peroxide	-8.58
hydrogen sulfide	-0.70
isopropanol	-4.76
isopropyl ether	-0.53
m-cresol	-5.49
methane	2.00
methanethiol	-1.24
methanol	-5.11
methyl 3-methyl-4-thiomethoxyphenyl thiophosphate	-6.92
methyl acetate	-3.32
methyl benzoate	-3.91
methyl butanoate	-2.83
methyl formate	-2.78
methyl hexanoate	-2.49
methyl isopropyl ether	-2.01
methyl octanoate	-2.04
methyl pentanoate	-2.57
methyl peroxide	-5.28
methyl propanoate	-2.93
methyl propyl ether	-1.66
methylamine	-4.56
methylcyclohexane	1.71
methylhydrazine	-5.31
m-hydroxybenzaldehyde	-9.51
morpholine	-7.17

m-xylene	-0.84
N,N-dimethylaniline	-3.58
N,N'-dimethylpiperazine	-7.58
naphthalene	-2.39
n-butane	2.08
N-ethylaniline	-4.62
n-heptane	2.62
n-hexane	2.49
nitrobenzene	-4.12
nitroethane	-3.71
nitromethane	-3.95
N-methylacetamide	-10.00
N-methylacetamide	-10.00
N-methylaniline	-4.68
N-methylmorpholine	-6.34
N-methylpiperazine	-7.77
n-octane	2.89
n-pentane	2.33
n-propane	1.96
o-chlorotoluene	-1.15
o-cresol	-5.87
octafluoropropane	4.28
octanal	-2.29
O-ethyl O'-4-bromo-2-chlorophenyl S-propyl phosphorothioate	-4.09
o-xylene	-0.90
p-bromophenol	-7.13
p-bromotoluene	-1.39
p-cresol	-6.14
p-dibromobenzene	-2.30
pentanal	-3.03
pentanoic acid	-6.16
pentyl acetate	-2.45
pentylamine	-4.10
phenol	-6.62
phosphine	0.60
p-hydroxybenzaldehyde	-10.48
piperazine	-7.40
piperidine	-5.11
propanal	-3.44
propanoic acid	-6.47
propene	1.27
propionitrile	-3.85
propyl acetate	-2.86
propylamine	-4.39
propyne	-0.31
p-xylene	-0.81
pyridine	-4.70
pyrrolidine	-5.48
s-trans-1,3-butadiene	0.61
t-butanol	-4.51
t-butyl methyl ether	-2.21
tetrachloroethene	0.05
tetrafluoromethane	3.16
tetrahydrofuran	-3.47
tetrahydropyran	-3.12
tetramethylsilane	3.04
thioanisole	-2.73
thiophene	-1.42
thiophenol	-2.55
toluene	-0.89
tribromomethane	-1.98
trichloroethene	-0.39
triethylphosphate	-7.80
trimethylamine	-3.23
trimethylphosphate	-8.70
tripropylphosphate	-6.10
urea	-13.80
water	-6.31
water dimer	-11.27

Table S2. Reference Solvation Free Energies (kcal/mol) for 66 Neutral Solutes in Water

From Nicholls et al., *J. Med. Chem.* **2008**, *51*, 769:

solute	free energy of solvation
1,1-diacetoxyethane	-4.97
1,1-diethoxyethane	-3.28
1,2-diethoxyethane	-3.54
1,3-diacetyloxypropan-2-yl acetate (glycerol triacetate)	-8.84
bis(2-chloroethyl) ether	-4.23
diethyl propanedioate	-6.00
dimethoxymethane	-2.93
ethylene glycol diacetate	-6.34
imidazole	-9.81
m-bis(trifluoromethyl) benzene	1.07
N,N,4-trimethylbenzamide	-9.76
N,N-dimethyl-p-methoxybenzamide	-11.01
phenyl formate	-3.82

From Guthrie, *J. Phys. Chem. B* **2009**, *113*, 4501:

solute	free energy of solvation
(2-dimethylamino-5,6-dimethyl-pyrimidin-4-yl) N,N-dimethylcarbamate (pirimor, pirimicarb)	-9.4
(RS)-2-sec-butyl-4,6-dinitrophenol (dinoseb)	-6.2
1,2,3,4,5,6-hexachlorocyclohexane (lindane)	-5.4
1,2-dinitroxypropane	-5.0
1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-4,7-methanoindene (heptachlor)	-2.6
1,4,5,8-tetraminoanthraquinone	-8.9
1-amino-4-anilinoanthraquinone	-7.4
1-amino-anthraquinone	-8.0
1-naphthyl methylcarbamate (carbaryl)	-9.5
2-(dimethoxyphosphinothioylthio) butanedioic acid diethyl ester (malathion)	-8.2
2-(ethylamino)-4-isopropylamino-6-methyl-thio-s-triazine (ametryn)	-7.7
2,3-dihydro-2,2-dimethyl-7-benzofuranyl methylcarbamate (carbofuran)	-9.6
2-butyl nitrate	-1.8
2-chloro-N-(2,6-diethylphenyl)-N-(methoxymethyl)acetamide (alachlor)	-8.2
2-methyl-2-(methylthio)propanal O-(N-methylcarbamoyl)oxime (aldicarb)	-9.8
3,5,5-trimethyl-2-cyclohexen-1-one (isophorone)	-5.2
3,6-dichloro-2-methoxybenzoic acid (dicamba)	-9.9
3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]- 1H-isoindole-1,3(2H)-dione (captan)	-9.0
3-t-butyl-5-chloro-6-methyluracil (terbacil)	-11.1
4-amino-4'-nitroazobenzene	-11.2
4-mesyl-2,6-dinitro-N,N-dipropylaniline (nitralin)	-8.0
5-amino-4-chloro-2-phenyl-3-(2H)-pyridazinone (pyrazon)	-16.4
5-Bromo-3-sec-butyl-6-methyl-uracil (bromacil)	-9.7
6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3-benzodioxathiepine-3-oxide	-4.2
6-chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine (simazine)	-10.2
a,a,a-trifluoro-2,6-dinitro-N,N-dipropyl-p-toluidine (trifluralin)	-3.3
butyl nitrate	-2.1
diethoxy-[(2-isopropyl-6-methyl-4-pyrimidinyl)oxy]-thioxophosphorane (diazinon)	-6.5
dimethyl (RS)-2,2,2-trichloro-1-hydroxyethylphosphonate (trichlorfon)	-12.7
endrin	-5.5
ethylene glycol mononitrate	-8.2
isobutyl nitrate	-1.9
N-(3,4-dichlorophenyl)propanamide (propanil)	-7.8
N1,N1-diethyl-2,6-dinitro-4-trifluoromethyl-m-phenylenediamine (dinitramine)	-5.7
N2,N4-diisopropyl-6-methylthio-1,3,5-triazine-2,4-diamine (prometryn)	-8.4
N2-tert-butyl-N4-ethyl-6-methylthio-1,3,5-triazine-2,4-diamine (terbutryn)	-6.7
N-butyl-N-ethyl-2,6-dinitro-4-(trifluoromethyl)aniline (benefin)	-3.5
N-cyclopropylmethyl-2,6-dinitro-N-propyl-4-trifluoromethylaniline (profluralin)	-2.5
nitroglycol	-5.7
nitroxyacetone	-6.0
N-methylcarbamic acid [1-(methylthio)ethylideneamino] ester (methomyl)	-10.7
O,O,O',O'-tetraethyl S,S'-methylene bis(phosphorodithioate) (ethion)	-6.1
O,O-diethyl O-3,5,6-trichloro-2-pyridyl phosphorothioate (chlorpyrifos)	-5.0
O,O-diethyl S-ethylthiomethyl phosphorodithioate (phorate)	-4.4
O,O-diethyl-O-4-nitro-phenylthiophosphate (parathion)	-6.7
O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] dithiophosphate	-10.0

octachloro-4,7-methanohydroindane (chlordane)	-3.4
phosphoric acid [(E)-2-chloro-1-(2,4-dichlorophenyl)vinyl] diethyl ester (chlorfenvinphos)	-7.1
S-(RS)-2-chloro-1-phthalimidoethyl O,O-diethyl phosphorodithioate (dialifor)	-5.7
S-4-chlorophenylthiomethyl O,O-diethyl phosphorodithioate (carbophenothion)	-6.5
S-propyl butyl(ethyl)thiocarbamate (pebulate)	-3.6
S-propyl dipropyl(thiocarbamate) (vernolate)	-4.1
trichloro(nitro)methane (chloropicrin)	-1.5

Table S3. Reference Solvation Free Energies (kcal/mol) for 26 Neutral Solutes in Water

Geballe et al., *J. Comput. Aided Mol. Des.* **2010**, *24*, 259:

solute	**free energy of solvation**
acetylsalicylic acid	-9.94
5-bromouracil	-18.17
butylparaben	-8.72
caffeine	-12.64
5-chlorouracil	-17.74
6-chlorouracil	-15.83
cyanuric acid	-18.06
diflunisal	-9.40
ethylparaben	-9.20
5-fluorouracil	-16.92
flurbiprofen (racemic)	-8.42
hexachlorobenzene	-2.33
ibuprofen (racemic)	-7.00
5-iodouracil	-18.72
ketoprofen (racemic)	-10.78
methylparaben	-9.51
naproxen	-10.21
4-nitroaniline	-9.45
octafluorocyclobutane	3.43
pentachloronitrobenzene	-5.22
phthalimide	-9.61
propylparaben	-9.37
sulfolane	-8.61
trimethyl *o*-trifluoroacetate	-0.80
5-(trifluoromethyl)uracil	-15.46
uracil	-16.59

Table S4. Reference Solvation Free Energies (kcal/mol) for 8 Iodine-Containing Hydrocarbons in Water

Zhu et. al., *J. Chem. Phys*. **1998**, *109*, 9117:

solute	free energy of solvation
1-iodobutane	-0.25
1-iodobutane	-0.25
1-iodopentane	-0.12
1-iodopentane	-0.12
1-iodopropane	-0.59
1-iodopropane	-0.59
2-iodopropane	-0.46
2-iodopropane	-0.46
diiodomethane	-2.49
diiodomethane	-2.49
iodobenzene	-1.73
iodoethane	-0.72
iodoethane	-0.72
iodomethane	-0.89
iodomethane	-0.89

Table S5. 2129 Reference Solvation Free Energies (kcal/mol) for 310 Neutral Solutes in 90 Organic Solvents

2072 nonaqueous data taken from the SM8/SMD/SM8AD training set:

solute	solvent keyword	free energy of solvation
1,4-dioxane	2methylpyridine	-5.01
2-butanone	2methylpyridine	-4.52
2-methylpyridine	2methylpyridine	-5.71
ethanol	2methylpyridine	-5.01
n-octane	2methylpyridine	-4.73
toluene	2methylpyridine	-5.06
4-methyl-2-pentanone	4methyl2pentanone	-5.23
acetic acid	4methyl2pentanone	-6.33
ammonia	4methyl2pentanone	-2.52
aniline	4methyl2pentanone	-7.54
butanoic acid	4methyl2pentanone	-7.44
diethylamine	4methyl2pentanone	-3.63
m-cresol	4methyl2pentanone	-8.79
methylamine	4methyl2pentanone	-4.14
naphthalene	4methyl2pentanone	-7.45
phenol	4methyl2pentanone	-9.38
propanoic acid	4methyl2pentanone	-6.85
pyridine	4methyl2pentanone	-5.33
trimethylamine	4methyl2pentanone	-2.86
1,4-dioxane	aceticacid	-5.80
2-butanone	aceticacid	-4.80
acetic acid	aceticacid	-5.30
ethanol	aceticacid	-5.25
nitromethane	aceticacid	-4.88
n-octane	aceticacid	-3.93
toluene	aceticacid	-4.53
1,4-dioxane	acetonitrile	-5.33
2-butanone	acetonitrile	-4.73
acetonitrile	acetonitrile	-4.85
ethanol	acetonitrile	-4.43
nitromethane	acetonitrile	-5.62
n-octane	acetonitrile	-3.57
toluene	acetonitrile	-4.68
1,4-dioxane	acetophenone	-5.03
2-butanone	acetophenone	-4.39
acetic acid	acetophenone	-6.20
acetophenone	acetophenone	-7.59
ethanol	acetophenone	-4.12
hydrogen peroxide	acetophenone	-7.30
nitromethane	acetophenone	-4.92
n-octane	acetophenone	-4.24
toluene	acetophenone	-4.90
1,4-dioxane	aniline	-5.65
2-butanone	aniline	-4.87
acetic acid	aniline	-6.30
aniline	aniline	-7.61
ethanol	aniline	-4.45
hydrogen peroxide	aniline	-7.80
nitromethane	aniline	-5.11
n-octane	aniline	-3.48
propanoic acid	aniline	-6.20
toluene	aniline	-4.57
1,4-dioxane	anisole	-5.06
2-butanone	anisole	-4.43
anisole	anisole	-6.33
butylamine	anisole	-4.44
ethanol	anisole	-3.59
nitromethane	anisole	-4.69
n-octane	anisole	-4.62
toluene	anisole	-4.95
1,1-dimethyl-3-phenylurea	benzene	-12.18
1,4-dioxane	benzene	-5.21

1-butanol	benzene	-4.45
1-heptanol	benzene	-6.85
1-hexanol	benzene	-6.13
1-octanol	benzene	-8.06
1-pentanol	benzene	-5.10
1-propanol	benzene	-3.87
2,2-dichloroethenyl dimethyl phosphate	benzene	-9.09
2,6-dimethylpyridine	benzene	-6.39
2-butanone	benzene	-4.46
2-heptanone	benzene	-6.36
2-hexanone	benzene	-5.76
2-methylaniline	benzene	-7.37
2-methylpyridine	benzene	-5.86
2-pentanone	benzene	-5.14
3,5-dimethylpyridine	benzene	-7.64
3-methylaniline	benzene	-7.61
4-methylaniline	benzene	-7.59
4-methylpyridine	benzene	-6.17
acetic acid	benzene	-4.02
acetone	benzene	-3.79
ammonia	benzene	-1.12
aniline	benzene	-6.88
benzamide	benzene	-9.93
benzene	benzene	-4.55
butanoic acid	benzene	-5.30
butyl acetate	benzene	-5.78
cyclohexane	benzene	-4.05
diethyl 4-nitrophenyl thiophosphonate	benzene	-8.58
diethylamine	benzene	-4.02
dimethyl 4-nitrophenyl thiophosphate	benzene	-9.21
dimethylamine	benzene	-3.01
dipropylamine	benzene	-5.09
ethanol	benzene	-3.42
ethyl acetate	benzene	-4.53
ethylamine	benzene	-2.73
hexanoic acid	benzene	-6.94
hydrazine	benzene	-4.02
hydrogen peroxide	benzene	-4.77
isopropanol	benzene	-3.48
m-cresol	benzene	-6.66
methanol	benzene	-2.58
methyl acetate	benzene	-4.04
methyl benzoate	benzene	-6.27
methyl hexanoate	benzene	-6.47
methyl pentanoate	benzene	-5.83
methyl propanoate	benzene	-4.58
methylamine	benzene	-2.66
m-hydroxybenzaldehyde	benzene	-9.29
n-hexane	benzene	-3.62
nitrobenzene	benzene	-7.60
nitromethane	benzene	-4.50
N-methylaniline	benzene	-6.64
n-octane	benzene	-5.35
n-pentane	benzene	-2.99
o-cresol	benzene	-7.44
p-bromophenol	benzene	-8.81
p-cresol	benzene	-7.35
pentanoic acid	benzene	-6.01
pentyl acetate	benzene	-6.53
phenol	benzene	-7.12
p-hydroxybenzaldehyde	benzene	-9.73
piperidine	benzene	-5.03
propanoic acid	benzene	-4.75
propyl acetate	benzene	-5.21
propylamine	benzene	-3.68
pyridine	benzene	-5.28
t-butanol	benzene	-3.70
toluene	benzene	-5.32
triethylphosphate	benzene	-8.58
trimethylamine	benzene	-2.80

trimethylphosphate	benzene	-8.02
tripropylphosphate	benzene	-9.34
water	benzene	-1.71
1,4-dioxane	benzonitrile	-5.14
2-butanone	benzonitrile	-4.58
benzonitrile	benzonitrile	-7.28
ethanol	benzonitrile	-4.05
nitromethane	benzonitrile	-5.05
n-octane	benzonitrile	-4.34
toluene	benzonitrile	-4.95
1,4-dioxane	benzylalcohol	-5.39
2-butanone	benzylalcohol	-4.57
acetic acid	benzylalcohol	-6.96
benzylalcohol	benzylalcohol	-8.61
butylamine	benzylalcohol	-5.15
ethanol	benzylalcohol	-4.84
formaldehyde	benzylalcohol	-3.48
nitromethane	benzylalcohol	-4.53
n-octane	benzylalcohol	-3.77
toluene	benzylalcohol	-4.46
1,4-dioxane	bromobenzene	-5.02
1-butanol	bromobenzene	-4.08
1-heptanol	bromobenzene	-6.68
1-hexanol	bromobenzene	-5.92
1-pentanol	bromobenzene	-5.06
1-propanol	bromobenzene	-3.74
2-butanone	bromobenzene	-4.37
4-methylaniline	bromobenzene	-7.59
aniline	bromobenzene	-6.66
bromobenzene	bromobenzene	-6.25
butyl acetate	bromobenzene	-5.58
butylamine	bromobenzene	-4.22
ethanol	bromobenzene	-3.26
ethyl acetate	bromobenzene	-4.57
ethylamine	bromobenzene	-2.73
methanol	bromobenzene	-2.31
methyl acetate	bromobenzene	-3.87
nitromethane	bromobenzene	-4.25
n-octane	bromobenzene	-5.02
o-cresol	bromobenzene	-6.87
o-cresol	bromobenzene	-7.26
p-bromophenol	bromobenzene	-8.49
p-cresol	bromobenzene	-7.12
pentyl acetate	bromobenzene	-6.35
propyl acetate	bromobenzene	-4.93
propylamine	bromobenzene	-3.57
toluene	bromobenzene	-5.13
1,4-dioxane	bromoethane	-5.39
2-butanone	bromoethane	-5.13
bromoethane	bromoethane	-3.67
nitromethane	bromoethane	-4.54
n-octane	bromoethane	-5.54
propanoic acid	bromoethane	-5.52
toluene	bromoethane	-5.55
1-butanol	bromoform	-4.72
1-heptanol	bromoform	-7.10
1-hexanol	bromoform	-6.20
1-pentanol	bromoform	-5.34
1-propanol	bromoform	-4.03
acetic acid	bromoform	-4.54
bromoform	bromoform	-6.21
ethanol	bromoform	-3.24
methanol	bromoform	-2.79
o-cresol	bromoform	-7.45
p-bromophenol	bromoform	-8.49
phenol	bromoform	-6.88
butyl acetate	bromooctane	-5.11
ethyl acetate	bromooctane	-3.97
methyl acetate	bromooctane	-3.35
pentyl acetate	bromooctane	-5.81

propyl acetate	bromooctane	-4.48
1,2-ethanediol	butanol	-8.69
1-butanol	butanol	-6.03
2-butanone	butanol	-4.12
acetic acid	butanol	-6.81
benzene	butanol	-3.39
butanoic acid	butanol	-7.66
diethylamine	butanol	-5.15
ethanol	butanol	-5.02
ethylamine	butanol	-4.50
ethylbenzene	butanol	-4.46
formaldehyde	butanol	-3.49
hexanoic acid	butanol	-8.75
hydrogen peroxide	butanol	-7.94
methanol	butanol	-4.73
nitromethane	butanol	-3.93
n-octane	butanol	-4.45
pentanoic acid	butanol	-8.02
propanoic acid	butanol	-7.17
propylamine	butanol	-5.04
toluene	butanol	-4.50
1,4-dioxane	butanone	-5.02
2-butanone	butanone	-4.50
acetic acid	butanone	-6.88
butanoic acid	butanone	-7.34
ethanol	butanone	-4.46
formaldehyde	butanone	-1.77
g-butyrolactone	butanone	-4.47
hexanoic acid	butanone	-8.07
nitromethane	butanone	-5.24
n-octane	butanone	-4.64
pentanoic acid	butanone	-7.54
propanoic acid	butanone	-7.05
toluene	butanone	-5.06
1,2-ethanediol	butylacetate	-6.27
1-butanol	butylacetate	-5.23
1-heptanol	butylacetate	-7.14
1-hexanol	butylacetate	-6.62
1-octanol	butylacetate	-8.17
1-pentanol	butylacetate	-5.78
1-propanol	butylacetate	-4.52
4-methylaniline	butylacetate	-7.81
acetic acid	butylacetate	-6.11
aniline	butylacetate	-7.30
butyl acetate	butylacetate	-5.52
ethanol	butylacetate	-3.97
hydrogen peroxide	butylacetate	-6.76
m-cresol	butylacetate	-8.44
methanol	butylacetate	-3.04
naphthalene	butylacetate	-7.59
o-cresol	butylacetate	-8.90
p-bromophenol	butylacetate	-10.57
p-cresol	butylacetate	-9.28
phenol	butylacetate	-8.96
pyridine	butylacetate	-5.31
water	butylacetate	-4.13
2-heptanone	butylbenzene	-5.93
2-hexanone	butylbenzene	-5.31
2-pentanone	butylbenzene	-4.74
3,3-dimethylbutanone	butylbenzene	-4.77
butyl acetate	butylbenzene	-5.28
butylbenzene	butylbenzene	-6.86
methyl hexanoate	butylbenzene	-6.09
methyl pentanoate	butylbenzene	-5.37
methyl propanoate	butylbenzene	-4.19
phenol	butylbenzene	-6.76
1,4-dioxane	carbondisulfide	-4.67
1-nitropropane	carbondisulfide	-4.50
2-butanone	carbondisulfide	-3.85
acetic acid	carbondisulfide	-2.98

acetone	carbondisulfide	-3.14
carbondisulfide	carbondisulfide	-3.95
ethanol	carbondisulfide	-2.72
ethyl acetate	carbondisulfide	-4.08
hydrogen peroxide	carbondisulfide	-3.14
methyl acetate	carbondisulfide	-3.67
nitromethane	carbondisulfide	-3.30
n-octane	carbondisulfide	-5.68
o-cresol	carbondisulfide	-6.27
propyl acetate	carbondisulfide	-4.63
toluene	carbondisulfide	-5.39
1,4-dichlorobenzene	carbontet	-6.28
1,4-dioxane	carbontet	-4.97
1-butanol	carbontet	-4.20
1-butene	carbontet	-2.48
1-heptanol	carbontet	-6.49
1-hexanol	carbontet	-5.04
1-nitropropane	carbontet	-4.49
1-pentanol	carbontet	-4.73
1-propanol	carbontet	-3.64
2-butanone	carbontet	-4.09
2-heptanone	carbontet	-6.12
2-hexanone	carbontet	-5.47
2-methyl-1-nitrobenzene	carbontet	-7.49
2-methylaniline	carbontet	-7.16
2-methylpropene	carbontet	-2.63
2-pentanone	carbontet	-4.81
2-pentene	carbontet	-3.46
3-methylaniline	carbontet	-7.23
4-methylaniline	carbontet	-7.24
acetic acid	carbontet	-3.64
acetone	carbontet	-3.35
acetophenone	carbontet	-7.10
ammonia	carbontet	-1.06
aniline	carbontet	-6.10
anisole	carbontet	-5.49
benzaldehyde	carbontet	-6.11
benzamide	carbontet	-9.13
benzene	carbontet	-4.50
benzonitrile	carbontet	-6.28
bromobenzene	carbontet	-5.85
butanoic acid	carbontet	-4.81
butyl acetate	carbontet	-5.59
butylamine	carbontet	-5.35
carbontet	carbontet	-4.35
chlorobenzene	carbontet	-5.21
cyclopentanone	carbontet	-5.26
diethylamine	carbontet	-4.12
dimethylamine	carbontet	-2.75
ethanol	carbontet	-2.96
ethyl acetate	carbontet	-4.40
ethylamine	carbontet	-2.77
ethylbenzene	carbontet	-5.67
fluorobenzene	carbontet	-3.64
hexanoic acid	carbontet	-6.99
hydrogen peroxide	carbontet	-3.14
isopropanol	carbontet	-3.15
methanol	carbontet	-2.25
methyl acetate	carbontet	-3.82
methyl benzoate	carbontet	-7.19
methyl hexanoate	carbontet	-6.39
methyl pentanoate	carbontet	-5.71
methyl propanoate	carbontet	-4.43
methylamine	carbontet	-2.53
m-xylene	carbontet	-5.71
naphthalene	carbontet	-7.55
nitrobenzene	carbontet	-6.92
nitromethane	carbontet	-3.52
N-methylaniline	carbontet	-6.58
n-octane	carbontet	-5.39

o-cresol	carbontet	-6.51
o-xylene	carbontet	-6.07
p-bromophenol	carbontet	-7.86
p-cresol	carbontet	-6.32
pentyl acetate	carbontet	-6.35
phenol	carbontet	-6.14
p-hydroxybenzaldehyde	carbontet	-8.16
propanoic acid	carbontet	-4.09
propyl acetate	carbontet	-5.03
propylamine	carbontet	-3.59
pyridine	carbontet	-5.01
t-butanol	carbontet	-3.40
thioanisole	carbontet	-5.66
toluene	carbontet	-5.12
triethylphosphate	carbontet	-7.51
trimethylamine	carbontet	-3.09
trimethylphosphate	carbontet	-7.24
tripropylphosphate	carbontet	-8.60
water	carbontet	-0.85
1,4-dioxane	chlorobenzene	-5.08
1-butanol	chlorobenzene	-4.31
1-heptanol	chlorobenzene	-6.78
1-hexanol	chlorobenzene	-5.98
1-pentanol	chlorobenzene	-5.25
1-propanol	chlorobenzene	-3.82
2-butanone	chlorobenzene	-4.47
2-heptanone	chlorobenzene	-6.46
2-hexanone	chlorobenzene	-5.84
2-pentanone	chlorobenzene	-5.29
3,3-dimethylbutanone	chlorobenzene	-5.25
4-methylaniline	chlorobenzene	-7.54
acetone	chlorobenzene	-3.86
ammonia	chlorobenzene	-1.22
aniline	chlorobenzene	-6.72
butyl acetate	chlorobenzene	-5.74
chlorobenzene	chlorobenzene	-5.66
dimethylamine	chlorobenzene	-2.75
ethanol	chlorobenzene	-3.30
ethyl acetate	chlorobenzene	-4.63
ethylamine	chlorobenzene	-2.73
methanol	chlorobenzene	-2.44
methyl acetate	chlorobenzene	-4.00
methyl pentanoate	chlorobenzene	-5.83
methyl propanoate	chlorobenzene	-4.55
methylamine	chlorobenzene	-2.16
nitromethane	chlorobenzene	-4.32
n-octane	chlorobenzene	-5.16
o-cresol	chlorobenzene	-6.96
o-cresol	chlorobenzene	-7.33
p-bromophenol	chlorobenzene	-8.54
p-cresol	chlorobenzene	-7.23
pentyl acetate	chlorobenzene	-6.49
propanoic acid	chlorobenzene	-4.38
propyl acetate	chlorobenzene	-5.15
propylamine	chlorobenzene	-3.59
toluene	chlorobenzene	-5.18
trimethylamine	chlorobenzene	-2.82
1,1-dimethyl-3-phenylurea	chloroform	-13.64
1,2-ethanediol	chloroform	-5.98
1,4-dichlorobenzene	chloroform	-6.32
1,4-dioxane	chloroform	-6.21
1-butanol	chloroform	-5.28
1-heptanol	chloroform	-7.53
1-hexanol	chloroform	-6.67
1-methylthymine	chloroform	-9.71
1-pentanol	chloroform	-5.90
1-propanol	chloroform	-4.41
2,2,2-trifluoroethanol	chloroform	-3.03
2,6-dimethylpyridine	chloroform	-7.74
2-butanone	chloroform	-5.43

2-ethylpyrazine	chloroform	-7.72
2-methyl-1-nitrobenzene	chloroform	-8.30
2-methylaniline	chloroform	-8.23
2-methylpyrazine	chloroform	-6.99
2-methylpyridine	chloroform	-6.98
3-methylpyridine	chloroform	-7.35
4-methylaniline	chloroform	-8.01
4-methylpyridine	chloroform	-7.50
9-methyladenine	chloroform	-12.51
acetaldehyde	chloroform	-3.65
acetamide	chloroform	-7.05
acetic acid	chloroform	-4.74
acetone	chloroform	-4.42
acetonitrile	chloroform	-4.44
acetophenone	chloroform	-7.81
allyl alcohol	chloroform	-4.34
ammonia	chloroform	-2.41
aniline	chloroform	-7.34
anisole	chloroform	-6.24
benzaldehyde	chloroform	-7.09
benzamide	chloroform	-11.06
benzene	chloroform	-4.64
benzonitrile	chloroform	-7.22
bromobenzene	chloroform	-6.07
butanoic acid	chloroform	-5.99
butyl acetate	chloroform	-6.71
chlorobenzene	chloroform	-5.45
chloroform	chloroform	-4.13
cyclohexane	chloroform	-4.45
diethyl ether	chloroform	-4.32
diethyl sulfide	chloroform	-6.40
diethylamine	chloroform	-5.23
difluorodichloromethane	chloroform	-1.55
dimethyl 4-nitrophenyl thiophosphate	chloroform	-9.51
dimethylamine	chloroform	-3.69
ethanol	chloroform	-3.94
ethyl acetate	chloroform	-5.58
ethyl phenyl ether	chloroform	-7.16
ethylamine	chloroform	-4.02
ethylbenzene	chloroform	-5.84
fluorobenzene	chloroform	-4.25
fluorotrichloromethane	chloroform	-2.62
formaldehyde	chloroform	0.12
hexanoic acid	chloroform	-7.51
hydrazine	chloroform	-4.42
hydrogen peroxide	chloroform	-4.70
hydrogen sulfide	chloroform	-0.51
isopropanol	chloroform	-4.28
isopropyl ether	chloroform	-3.78
m-cresol	chloroform	-6.70
methanol	chloroform	-3.32
methyl acetate	chloroform	-4.90
methyl benzoate	chloroform	-7.81
methyl hexanoate	chloroform	-7.24
methyl pentanoate	chloroform	-6.68
methyl propanoate	chloroform	-5.48
methylamine	chloroform	-3.17
morpholine	chloroform	-6.72
m-xylene	chloroform	-5.86
N,N-dimethylacetamide	chloroform	-8.38
naphthalene	chloroform	-7.89
nitrobenzene	chloroform	-7.78
nitromethane	chloroform	-4.68
N-methyl-2-pyrrolidinone	chloroform	-9.82
n-octane	chloroform	-5.25
o-cresol	chloroform	-7.55
o-xylene	chloroform	-6.23
p-bromophenol	chloroform	-8.59
p-cresol	chloroform	-7.59
pentanoic acid	chloroform	-6.61

pentyl acetate	chloroform	-7.36
phenol	chloroform	-7.14
p-hydroxybenzaldehyde	chloroform	-10.30
piperidine	chloroform	-6.37
propanoic acid	chloroform	-5.37
propyl acetate	chloroform	-6.35
propylamine	chloroform	-4.73
pyridine	chloroform	-6.45
pyrrole	chloroform	-5.50
quinoline	chloroform	-10.23
t-butanol	chloroform	-4.48
tetrahydropyran	chloroform	-5.84
thioanisole	chloroform	-5.98
thiophene	chloroform	-5.83
thiophenol	chloroform	-7.61
toluene	chloroform	-5.48
triethylphosphate	chloroform	-10.90
trimethylamine	chloroform	-3.90
trimethylphosphate	chloroform	-9.74
tripropylphosphate	chloroform	-11.11
urea	chloroform	-8.56
water	chloroform	-2.05
2-butanone	chlorohexane	-4.10
2-hexanone	chlorohexane	-5.42
2-pentanone	chlorohexane	-4.84
3,3-dimethylbutanone	chlorohexane	-4.98
acetone	chlorohexane	-3.45
butyl acetate	chlorohexane	-5.37
ethyl acetate	chlorohexane	-4.25
methyl acetate	chlorohexane	-3.66
methyl pentanoate	chlorohexane	-5.41
methyl propanoate	chlorohexane	-4.20
propyl acetate	chlorohexane	-4.84
1,1,1-trichloroethane	cyclohexane	-4.08
1,4-dichlorobenzene	cyclohexane	-5.89
1,4-dioxane	cyclohexane	-4.17
1-butanol	cyclohexane	-3.52
1-heptanol	cyclohexane	-6.02
1-hexanol	cyclohexane	-5.31
1-nitropropane	cyclohexane	-4.06
1-pentanol	cyclohexane	-3.61
1-propanethiol	cyclohexane	-3.12
1-propanol	cyclohexane	-2.73
2,2,2-trifluoroethanol	cyclohexane	-1.53
2,6-dimethylpyridine	cyclohexane	-5.51
2-butanone	cyclohexane	-3.48
2-heptanone	cyclohexane	-5.47
2-hexanone	cyclohexane	-4.77
2-methyl-1-nitrobenzene	cyclohexane	-6.71
2-methylaniline	cyclohexane	-6.44
2-methylpyridine	cyclohexane	-5.05
2-pentanone	cyclohexane	-4.19
3,3-dimethylbutanone	cyclohexane	-4.42
3,5-dibromo-4-hydroxybenzonitrile	cyclohexane	-6.83
3-methylaniline	cyclohexane	-6.47
3-methylpyridine	cyclohexane	-5.14
3-pentanone	cyclohexane	-4.30
4-methylaniline	cyclohexane	-6.30
4-methylpyridine	cyclohexane	-5.23
acetic acid	cyclohexane	-1.73
acetone	cyclohexane	-2.67
acetonitrile	cyclohexane	-1.87
acetophenone	cyclohexane	-6.29
aniline	cyclohexane	-5.52
anisole	cyclohexane	-5.38
benzaldehyde	cyclohexane	-5.71
benzamide	cyclohexane	-8.72
benzene	cyclohexane	-4.19
benzonitrile	cyclohexane	-5.54
bromobenzene	cyclohexane	-5.29

butyl acetate	cyclohexane	-4.94
chlorobenzene	cyclohexane	-5.10
cyclohexane	cyclohexane	-4.43
diethyl ether	cyclohexane	-3.03
diethylamine	cyclohexane	-3.61
difluorodichloromethane	cyclohexane	-1.81
ethanol	cyclohexane	-2.42
ethyl acetate	cyclohexane	-3.56
ethyl phenyl ether	cyclohexane	-6.00
ethylamine	cyclohexane	-2.04
ethylbenzene	cyclohexane	-4.97
fluorobenzene	cyclohexane	-3.59
fluorotrichloromethane	cyclohexane	-2.63
isopropanol	cyclohexane	-2.37
m-cresol	cyclohexane	-5.20
methanol	cyclohexane	-1.29
methyl acetate	cyclohexane	-3.06
methyl benzoate	cyclohexane	-7.01
methyl hexanoate	cyclohexane	-5.75
methyl pentanoate	cyclohexane	-5.04
methyl propanoate	cyclohexane	-3.71
m-hydroxybenzaldehyde	cyclohexane	-6.88
m-xylene	cyclohexane	-5.52
N,N-dimethylformamide	cyclohexane	-3.82
naphthalene	cyclohexane	-7.17
n-butane	cyclohexane	-2.86
nitrobenzene	cyclohexane	-6.62
nitromethane	cyclohexane	-2.86
N-methylaniline	cyclohexane	-6.33
n-octane	cyclohexane	-5.63
n-pentane	cyclohexane	-3.50
n-propane	cyclohexane	-2.09
o-cresol	cyclohexane	-6.02
o-xylene	cyclohexane	-5.54
p-bromophenol	cyclohexane	-7.14
p-cresol	cyclohexane	-5.89
pentyl acetate	cyclohexane	-5.71
phenol	cyclohexane	-5.57
p-hydroxybenzaldehyde	cyclohexane	-7.19
propanoic acid	cyclohexane	-3.78
propyl acetate	cyclohexane	-4.36
pyridine	cyclohexane	-4.30
pyrrole	cyclohexane	-3.77
quinoline	cyclohexane	-7.38
t-butanol	cyclohexane	-2.93
tetrahydropyran	cyclohexane	-4.41
thioanisole	cyclohexane	-5.66
toluene	cyclohexane	-4.90
trichloroethene	cyclohexane	-4.29
triethylphosphate	cyclohexane	-7.60
trimethylamine	cyclohexane	-2.63
trimethylphosphate	cyclohexane	-5.67
tripropylphosphate	cyclohexane	-7.71
water	cyclohexane	-0.39
1,4-dioxane	cyclohexanone	-4.95
2-butanone	cyclohexanone	-4.42
acetic acid	cyclohexanone	-6.43
cyclohexanone	cyclohexanone	-6.25
ethanol	cyclohexanone	-4.41
hydrogen peroxide	cyclohexanone	-9.11
nitromethane	cyclohexanone	-5.09
n-octane	cyclohexanone	-4.57
propanoic acid	cyclohexanone	-7.18
toluene	cyclohexanone	-5.05
acetic acid	decalin	-4.49
acetophenone	decalin	-6.23
aniline	decalin	-5.78
anisole	decalin	-5.00
benzonitrile	decalin	-5.86
bromobenzene	decalin	-5.25

butyl acetate	decalin	-4.71
butylamine	decalin	-3.72
chlorobenzene	decalin	-4.61
ethyl acetate	decalin	-3.47
fluorobenzene	decalin	-3.44
m-cresol	decalin	-5.11
methyl acetate	decalin	-2.90
methyl benzoate	decalin	-6.76
methyl hexanoate	decalin	-5.51
methyl pentanoate	decalin	-4.83
methyl propanoate	decalin	-3.50
nitrobenzene	decalin	-6.36
N-methylaniline	decalin	-6.41
p-cresol	decalin	-5.68
pentyl acetate	decalin	-5.44
phenol	decalin	-5.38
propanoic acid	decalin	-4.42
propyl acetate	decalin	-4.05
thioanisole	decalin	-5.54
toluene	decalin	-4.37
1,4-dioxane	decane	-3.97
1-butanol	decane	-3.77
1-heptanol	decane	-5.62
1-hexanol	decane	-4.97
1-pentanol	decane	-3.92
1-propanol	decane	-2.76
2-butanone	decane	-3.30
2-heptanone	decane	-5.18
2-hexanone	decane	-4.61
2-pentanone	decane	-3.93
3,3-dimethylbutanone	decane	-4.15
4-methylaniline	decane	-6.05
acetamide	decane	-2.85
acetone	decane	-2.47
benzene	decane	-3.80
bromobenzene	decane	-5.43
butyl acetate	decane	-4.66
butylamine	decane	-3.55
chlorobenzene	decane	-4.93
ethanol	decane	-2.44
ethyl acetate	decane	-3.43
ethylamine	decane	-1.92
ethylbenzene	decane	-5.25
fluorobenzene	decane	-3.48
methanol	decane	-1.29
methyl acetate	decane	-2.98
methyl hexanoate	decane	-5.48
methyl pentanoate	decane	-4.77
methyl propanoate	decane	-3.49
n-decane	decane	-6.53
nitromethane	decane	-2.81
n-octane	decane	-5.18
p-cresol	decane	-6.00
pentyl acetate	decane	-5.31
phenol	decane	-5.50
propyl acetate	decane	-4.02
propylamine	decane	-2.96
toluene	decane	-4.65
trichloroethene	decane	-3.84
1-decanol	decanol	-9.58
2-methoxyethanol	decanol	-5.41
butylamine	decanol	-5.22
chlorobenzene	decanol	-4.83
ethylamine	decanol	-3.91
m-cresol	decanol	-8.01
o-cresol	decanol	-8.58
p-bromophenol	decanol	-10.32
p-cresol	decanol	-8.91
phenol	decanol	-8.58
propylamine	decanol	-4.59

1-butanol	dibromoethane	-4.65
1-heptanol	dibromoethane	-6.64
1-hexanol	dibromoethane	-6.08
1-pentanol	dibromoethane	-5.44
1-propanol	dibromoethane	-3.82
ethanol	dibromoethane	-2.69
methanol	dibromoethane	-2.38
p-bromophenol	dibromoethane	-9.01
p-cresol	dibromoethane	-7.52
phenol	dibromoethane	-7.22
1,4-dioxane	dibutylether	-4.37
2-butanone	dibutylether	-3.78
2-ethylpyrazine	dibutylether	-5.87
2-methylpyrazine	dibutylether	-5.12
2-methylpyridine	dibutylether	-5.20
acetic acid	dibutylether	-5.21
dibutylether	dibutylether	-5.76
diethylamine	dibutylether	-3.80
ethanol	dibutylether	-3.51
hydrogen peroxide	dibutylether	-5.75
nitromethane	dibutylether	-3.67
n-octane	dibutylether	-5.24
propanoic acid	dibutylether	-6.11
pyridine	dibutylether	-4.65
toluene	dibutylether	-4.87
1-butanol	dichloroethane	-4.92
1-heptanol	dichloroethane	-6.79
1-hexanol	dichloroethane	-6.02
1-pentanol	dichloroethane	-5.45
1-propanol	dichloroethane	-3.85
acetic acid	dichloroethane	-4.89
acetophenone	dichloroethane	-7.83
aniline	dichloroethane	-7.39
benzaldehyde	dichloroethane	-7.23
benzamide	dichloroethane	-10.90
butanoic acid	dichloroethane	-5.83
butyl acetate	dichloroethane	-5.93
butylamine	dichloroethane	-4.34
dichloroethane	dichloroethane	-4.69
diethylamine	dichloroethane	-4.00
ethanol	dichloroethane	-2.83
ethyl acetate	dichloroethane	-4.93
ethylamine	dichloroethane	-3.19
hexanoic acid	dichloroethane	-7.33
m-cresol	dichloroethane	-6.91
methanol	dichloroethane	-2.53
methyl acetate	dichloroethane	-4.55
methyl hexanoate	dichloroethane	-6.57
methyl pentanoate	dichloroethane	-5.97
methyl propanoate	dichloroethane	-4.87
m-hydroxybenzaldehyde	dichloroethane	-10.11
o-cresol	dichloroethane	-7.73
p-bromophenol	dichloroethane	-9.10
p-cresol	dichloroethane	-7.75
pentanoic acid	dichloroethane	-6.47
pentyl acetate	dichloroethane	-6.64
phenol	dichloroethane	-7.48
p-hydroxybenzaldehyde	dichloroethane	-10.70
propanoic acid	dichloroethane	-5.12
propyl acetate	dichloroethane	-5.40
propylamine	dichloroethane	-4.04
pyridine	dichloroethane	-5.53
triethylphosphate	dichloroethane	-9.59
trimethylphosphate	dichloroethane	-8.55
1,2-ethanediol	diethylether	-6.20
1,4-dichlorobenzene	diethylether	-6.18
1,4-dioxane	diethylether	-4.67
1-butanol	diethylether	-5.69
1-heptanol	diethylether	-7.51
1-hexanol	diethylether	-6.82

1-octanol	diethylether	-7.25
1-pentanol	diethylether	-6.11
1-propanol	diethylether	-4.90
2-butanone	diethylether	-4.09
2-methoxyethanol	diethylether	-5.12
2-methyl-1-nitrobenzene	diethylether	-7.21
acetaldehyde	diethylether	-2.85
acetamide	diethylether	-6.16
acetic acid	diethylether	-6.26
acetonitrile	diethylether	-3.59
acetophenone	diethylether	-6.79
allyl alcohol	diethylether	-4.87
ammonia	diethylether	-1.41
aniline	diethylether	-6.51
anisole	diethylether	-5.71
benzaldehyde	diethylether	-6.08
benzamide	diethylether	-10.60
benzene	diethylether	-4.21
benzonitrile	diethylether	-6.36
bromobenzene	diethylether	-5.99
butanoic acid	diethylether	-7.32
butylamine	diethylether	-4.24
chlorobenzene	diethylether	-5.42
cyclopentanol	diethylether	-6.50
diethyl ether	diethylether	-3.39
diethylamine	diethylether	-3.83
dimethylamine	diethylether	-2.63
dipropylamine	diethylether	-4.96
ethanol	diethylether	-4.41
ethylamine	diethylether	-2.89
ethylbenzene	diethylether	-5.45
formamide	diethylether	-5.97
hexanoic acid	diethylether	-8.85
hydrazine	diethylether	-3.08
hydrogen peroxide	diethylether	-7.03
hydrogen sulfide	diethylether	-0.60
isopropanol	diethylether	-4.44
m-cresol	diethylether	-7.95
methanol	diethylether	-3.61
methylamine	diethylether	-2.32
m-hydroxybenzaldehyde	diethylether	-11.36
m-xylene	diethylether	-5.56
N,N-dimethylformamide	diethylether	-5.31
naphthalene	diethylether	-7.25
nitrobenzene	diethylether	-6.85
nitromethane	diethylether	-4.19
n-octane	diethylether	-5.62
o-xylene	diethylether	-5.58
pentanoic acid	diethylether	-7.87
phenol	diethylether	-8.75
p-hydroxybenzaldehyde	diethylether	-12.07
piperidine	diethylether	-4.82
propanal	diethylether	-3.85
propanoic acid	diethylether	-6.75
propylamine	diethylether	-3.65
pyridine	diethylether	-4.81
t-butanol	diethylether	-4.80
toluene	diethylether	-5.23
trimethylamine	diethylether	-2.78
urea	diethylether	-9.11
water	diethylether	-3.85
1,4-dioxane	diisopropylether	-4.42
2-butanone	diisopropylether	-3.96
acetic acid	diisopropylether	-5.73
aniline	diisopropylether	-6.67
butanoic acid	diisopropylether	-6.85
diethylamine	diisopropylether	-3.78
ethanol	diisopropylether	-3.90
formaldehyde	diisopropylether	-1.04
hexanoic acid	diisopropylether	-8.23

hydrogen peroxide	diisopropylether	-6.72
isopropyl ether	diisopropylether	-3.97
naphthalene	diisopropylether	-7.24
nitromethane	diisopropylether	-3.90
n-octane	diisopropylether	-5.38
pentanoic acid	diisopropylether	-7.59
phenol	diisopropylether	-8.35
p-hydroxybenzaldehyde	diisopropylether	-11.63
propanoic acid	diisopropylether	-6.37
pyridine	diisopropylether	-4.88
toluene	diisopropylether	-4.91
trimethylamine	diisopropylether	-2.74
water	diisopropylether	-3.58
1,4-dioxane	dimethylacetamide	-5.01
2-butanone	dimethylacetamide	-4.52
ethanol	dimethylacetamide	-5.40
N,N-dimethylacetamide	dimethylacetamide	-6.77
nitromethane	dimethylacetamide	-5.62
n-octane	dimethylacetamide	-3.94
toluene	dimethylacetamide	-4.94
1,4-dioxane	dimethylformamide	-5.03
2-butanone	dimethylformamide	-4.56
ethanol	dimethylformamide	-5.23
N,N-dimethylformamide	dimethylformamide	-6.47
nitromethane	dimethylformamide	-5.66
n-octane	dimethylformamide	-3.77
toluene	dimethylformamide	-4.88
1,4-dioxane	dimethylpyridine	-4.90
2,6-dimethylpyridine	dimethylpyridine	-6.04
2-butanone	dimethylpyridine	-4.34
ethanol	dimethylpyridine	-4.87
n-octane	dimethylpyridine	-4.88
toluene	dimethylpyridine	-5.03
1,4-dioxane	DMSO	-4.90
2-butanone	DMSO	-4.23
DMSO	DMSO	-7.63
ethanol	DMSO	-5.25
nitromethane	DMSO	-5.66
n-octane	DMSO	-2.84
toluene	DMSO	-4.42
1-butanol	dodecane	-3.47
1-heptanol	dodecane	-5.41
1-hexanol	dodecane	-4.28
1-pentanol	dodecane	-4.09
1-propanol	dodecane	-2.74
acetophenone	dodecane	-6.11
ethanol	dodecane	-2.06
n-dodecane	dodecane	-7.83
1,4-dioxane	ethanol	-4.68
2-butanone	ethanol	-4.32
chlorobenzene	ethanol	-3.30
ethanol	ethanol	-5.04
g-butyrolactone	ethanol	-4.58
nitromethane	ethanol	-4.34
n-octane	ethanol	-4.23
toluene	ethanol	-4.57
1,4-dioxane	ethoxybenzene	-4.87
2-butanone	ethoxybenzene	-4.28
ethanol	ethoxybenzene	-3.45
ethyl phenyl ether	ethoxybenzene	-6.75
nitromethane	ethoxybenzene	-4.45
n-octane	ethoxybenzene	-4.75
toluene	ethoxybenzene	-4.99
1,2-ethanediol	ethylacetate	-6.82
1,4-dioxane	ethylacetate	-5.03
1-butanol	ethylacetate	-5.77
1-heptanol	ethylacetate	-7.56
1-hexanol	ethylacetate	-6.92
1-octanol	ethylacetate	-8.41
1-pentanol	ethylacetate	-6.13

1-propanol	ethylacetate	-4.90
4-methylaniline	ethylacetate	-7.63
acetic acid	ethylacetate	-6.46
butanoic acid	ethylacetate	-7.34
ethanol	ethylacetate	-4.24
ethyl acetate	ethylacetate	-4.46
hydrogen peroxide	ethylacetate	-7.60
methanol	ethylacetate	-3.37
nitromethane	ethylacetate	-5.06
n-octane	ethylacetate	-4.72
phenol	ethylacetate	-8.70
propanoic acid	ethylacetate	-6.95
toluene	ethylacetate	-5.05
water	ethylacetate	-4.26
1-butanol	ethylbenzene	-3.77
1-heptanol	ethylbenzene	-6.70
1-hexanol	ethylbenzene	-5.68
1-pentanol	ethylbenzene	-4.72
1-propanol	ethylbenzene	-3.71
2-butanone	ethylbenzene	-4.12
2-heptanone	ethylbenzene	-6.10
2-hexanone	ethylbenzene	-5.49
2-pentanone	ethylbenzene	-4.85
3,3-dimethylbutanone	ethylbenzene	-4.92
acetone	ethylbenzene	-3.41
butyl acetate	ethylbenzene	-5.48
butylamine	ethylbenzene	-4.43
ethanol	ethylbenzene	-2.49
ethyl acetate	ethylbenzene	-4.31
ethylamine	ethylbenzene	-2.59
ethylbenzene	ethylbenzene	-5.67
methanol	ethylbenzene	-1.43
methyl acetate	ethylbenzene	-3.74
methyl pentanoate	ethylbenzene	-5.56
methyl propanoate	ethylbenzene	-4.29
o-cresol	ethylbenzene	-7.25
p-bromophenol	ethylbenzene	-8.54
pentyl acetate	ethylbenzene	-6.20
phenol	ethylbenzene	-6.82
propyl acetate	ethylbenzene	-4.95
propylamine	ethylbenzene	-3.44
trimethylamine	ethylbenzene	-2.64
water	ethylbenzene	-1.51
1,4-dioxane	fluorobenzene	-5.18
2-butanone	fluorobenzene	-4.60
ethanol	fluorobenzene	-3.45
fluorobenzene	fluorobenzene	-4.60
nitromethane	fluorobenzene	-4.62
n-octane	fluorobenzene	-4.99
toluene	fluorobenzene	-5.27
butyl acetate	fluoroctane	-5.22
ethyl acetate	fluoroctane	-4.16
methyl acetate	fluoroctane	-3.59
methyl pentanoate	fluoroctane	-5.33
methyl propanoate	fluoroctane	-4.09
propyl acetate	fluoroctane	-4.65
1,2-dichlorobenzene	heptane	-6.01
1,4-dichlorobenzene	heptane	-5.81
1-butanol	heptane	-3.66
1-heptanol	heptane	-5.60
1-hexanol	heptane	-4.89
1-pentanol	heptane	-4.09
1-propanol	heptane	-3.01
2,2'-dichlorobiphenyl	heptane	-9.22
2-butanone	heptane	-3.36
2-heptanone	heptane	-5.22
2-hexanone	heptane	-4.55
2-methylaniline	heptane	-6.28
2-octanone	heptane	-5.68
2-pentanone	heptane	-4.07

3,3-dimethylbutanone	heptane	-4.30
3-methylaniline	heptane	-6.35
4-methylaniline	heptane	-6.15
acetone	heptane	-2.61
acetonitrile	heptane	-2.06
acetophenone	heptane	-6.14
aniline	heptane	-5.38
anisole	heptane	-5.35
anthracene	heptane	-10.00
benzaldehyde	heptane	-5.50
benzamide	heptane	-7.26
benzene	heptane	-4.00
benzonitrile	heptane	-5.33
bromobenzene	heptane	-5.72
butanoic acid	heptane	-5.05
butyl acetate	heptane	-4.83
butylamine	heptane	-3.55
chlorobenzene	heptane	-5.15
ethanol	heptane	-2.15
ethyl acetate	heptane	-3.50
ethylamine	heptane	-2.09
fluorobenzene	heptane	-4.13
hexanoic acid	heptane	-6.54
m-cresol	heptane	-5.01
methanol	heptane	-1.29
methyl acetate	heptane	-2.97
methyl hexanoate	heptane	-5.63
methyl pentanoate	heptane	-4.92
methyl propanoate	heptane	-3.63
m-xylene	heptane	-5.67
N,N-dimethylacetamide	heptane	-4.80
naphthalene	heptane	-7.02
n-heptane	heptane	-4.65
nitrobenzene	heptane	-6.14
N-methyl-2-pyrrolidinone	heptane	-5.80
o-cresol	heptane	-6.01
o-xylene	heptane	-5.52
p-cresol	heptane	-5.77
p-dibromobenzene	heptane	-7.55
pentanoic acid	heptane	-5.23
pentyl acetate	heptane	-5.42
phenol	heptane	-5.32
propanoic acid	heptane	-4.06
propyl acetate	heptane	-4.09
propylamine	heptane	-3.03
p-xylene	heptane	-5.52
pyridine	heptane	-4.28
thiophene	heptane	-4.09
toluene	heptane	-4.78
triethylphosphate	heptane	-6.67
trimethylphosphate	heptane	-5.59
tripropylphosphate	heptane	-7.50
1-heptanol	heptanol	-7.84
acetic acid	heptanol	-6.70
benzene	heptanol	-3.73
butylamine	heptanol	-5.40
ethylamine	heptanol	-4.15
ethylbenzene	heptanol	-4.58
o-cresol	heptanol	-8.78
p-bromophenol	heptanol	-10.49
p-cresol	heptanol	-9.16
phenol	heptanol	-8.69
propylamine	heptanol	-4.80
toluene	heptanol	-4.33
1,1,1-trichloroethane	hexadecane	-3.73
1,1,2-trichloro-1,2,2-trifluoroethane	hexadecane	-2.89
1,1,2-trichloroethane	hexadecane	-4.49
1,1-dichloro-2,2-difluoroethyl methyl ether	hexadecane	-3.90
1,2-dichlorobenzene	hexadecane	-6.16
1,2-dichloroethene	hexadecane	-3.11

1,2-dichloroethene	hexadecane	-3.33
1,2-dimethoxyethane	hexadecane	-3.63
1,2-ethanediol	hexadecane	-2.81
1,4-dichlorobenzene	hexadecane	-6.02
1,4-dioxane	hexadecane	-3.82
1-bromo-1,2,2,2-tetrafluoroethane	hexadecane	-1.87
1-bromo-1-chloro-2,2,2-trifluoroethane	hexadecane	-2.97
1-bromobutane	hexadecane	-4.24
1-bromo-isobutane	hexadecane	-4.04
1-bromopentane	hexadecane	-4.93
1-bromopropane	hexadecane	-3.57
1-butanol	hexadecane	-3.55
1-butene	hexadecane	-2.03
1-butyne	hexadecane	-2.07
1-chloropropane	hexadecane	-2.86
1-decanol	hexadecane	-7.68
1-fluorohexane	hexadecane	-4.03
1-fluorooctane	hexadecane	-5.25
1-heptanol	hexadecane	-5.62
1-hexanol	hexadecane	-4.92
1-hexene	hexadecane	-3.51
1-hexyne	hexadecane	-3.42
1-nitrobutane	hexadecane	-4.66
1-nitropropane	hexadecane	-3.95
1-octanol	hexadecane	-6.30
1-pentanol	hexadecane	-4.24
1-pentene	hexadecane	-2.79
1-pentyne	hexadecane	-2.74
1-propanethiol	hexadecane	-3.66
1-propanol	hexadecane	-2.77
2,2,2-trifluorethyl vinyl ether	hexadecane	-1.91
2,2,2-trifluoroethanol	hexadecane	-1.67
2,2,4-trimethylpentane	hexadecane	-4.24
2,2-dimethylpropane	hexadecane	-2.48
2,4-dimethylpentane	hexadecane	-3.87
2,4-dimethylpyridine	hexadecane	-5.52
2,5-dimethylpyridine	hexadecane	-5.52
2,6-dimethylpyridine	hexadecane	-5.27
2-bromopropane	hexadecane	-3.26
2-butanone	hexadecane	-3.12
2-chloropropane	hexadecane	-2.69
2-heptanone	hexadecane	-5.13
2-hexanone	hexadecane	-4.45
2-methyl-1-nitrobenzene	hexadecane	-6.52
2-methylaniline	hexadecane	-6.08
2-methylpentane	hexadecane	-3.48
2-methylpropane	hexadecane	-1.92
2-methylpyridine	hexadecane	-4.68
2-nitropropane	hexadecane	-3.47
2-octanone	hexadecane	-5.81
2-pentanone	hexadecane	-3.76
3,3-dimethylbutanone	hexadecane	-3.94
3,4-dimethylpyridine	hexadecane	-2.58
3,5-dimethylpyridine	hexadecane	-2.52
3-bromopropene	hexadecane	-3.42
3-chloropropene	hexadecane	-2.88
3-methylpyridine	hexadecane	-4.91
3-pentanone	hexadecane	-3.83
4-ethylpyridine	hexadecane	-2.45
4-heptanone	hexadecane	-5.20
4-methylaniline	hexadecane	-6.04
4-methylpyridine	hexadecane	-4.89
5-nonanone	hexadecane	-6.46
acetaldehyde	hexadecane	-1.68
acetamide	hexadecane	-3.33
acetic acid	hexadecane	-2.39
acetone	hexadecane	-2.31
acetonitrile	hexadecane	-2.37
acetophenone	hexadecane	-6.14
allyl alcohol	hexadecane	-2.73

ammonia	hexadecane	-0.93
aniline	hexadecane	-5.44
anisole	hexadecane	-5.35
anthracene	hexadecane	-10.32
benzaldehyde	hexadecane	-5.44
benzene	hexadecane	-3.80
benzonitrile	hexadecane	-5.51
bromobenzene	hexadecane	-5.51
bromoethane	hexadecane	-2.89
bromoform	hexadecane	-5.16
bromotoluene	hexadecane	-6.36
bromotrichloromethane	hexadecane	-4.46
butanal	hexadecane	-3.10
butanoic acid	hexadecane	-3.86
butanonitrile	hexadecane	-3.48
butyl acetate	hexadecane	-4.61
chlorobenzene	hexadecane	-4.99
chloroethane	hexadecane	-2.29
chloroform	hexadecane	-3.38
chrysene	hexadecane	-14.10
cyclohexane	hexadecane	-4.04
cyclopentane	hexadecane	-3.38
cyclopentanol	hexadecane	-4.42
cyclopentanone	hexadecane	-4.39
cyclopropane	hexadecane	-1.78
dibromomethane	hexadecane	-3.94
dichloromethane	hexadecane	-2.76
diethyl disulfide	hexadecane	-5.74
diethyl ether	hexadecane	-2.81
diethyl sulfide	hexadecane	-4.23
diethylamine	hexadecane	-3.27
dimethyl disulfide	hexadecane	-4.84
dimethyl ether	hexadecane	-1.49
dimethyl methylphosphonate	hexadecane	-5.43
dimethyl sulfide	hexadecane	-3.05
dimethylamine	hexadecane	-2.18
dipropyl sulfide	hexadecane	-5.61
dipropylamine	hexadecane	-4.57
ethane	hexadecane	-0.67
ethanethiol	hexadecane	-2.96
ethanol	hexadecane	-2.03
ethene	hexadecane	-0.39
ethyl acetate	hexadecane	-3.25
ethyl formate	hexadecane	-2.59
ethyl phenyl ether	hexadecane	-5.64
ethylamine	hexadecane	-2.29
ethylbenzene	hexadecane	-5.15
ethyloctadecanoate	hexadecane	-13.69
ethyne	hexadecane	-0.20
fluorobenzene	hexadecane	-4.03
fluoroethane	hexadecane	-0.76
formaldehyde	hexadecane	-0.99
formamide	hexadecane	-2.91
hexanoic acid	hexadecane	-5.35
hydrogen	hexadecane	1.64
hydrogen sulfide	hexadecane	-0.72
isopropanol	hexadecane	-2.47
isopropyl ether	hexadecane	-4.02
m-cresol	hexadecane	-5.91
methane	hexadecane	0.45
methanol	hexadecane	-1.32
methyl acetate	hexadecane	-2.67
methyl benzoate	hexadecane	-6.31
methyl butanoate	hexadecane	-4.01
methyl formate	hexadecane	-1.99
methyl hexanoate	hexadecane	-5.43
methyl pentanoate	hexadecane	-4.69
methyl propanoate	hexadecane	-2.68
methylcyclohexane	hexadecane	-4.43
m-xylene	hexadecane	-5.24

naphthalene	hexadecane	-7.29
n-butane	hexadecane	-2.20
n-heptane	hexadecane	-4.33
n-hexadecane	hexadecane	-10.52
n-hexane	hexadecane	-3.64
nitrobenzene	hexadecane	-6.22
nitroethane	hexadecane	-3.29
nitromethane	hexadecane	-2.58
N-methylaniline	hexadecane	-6.19
n-octane	hexadecane	-5.02
n-pentane	hexadecane	-2.95
n-propane	hexadecane	-1.43
o-cresol	hexadecane	-5.78
octanal	hexadecane	-5.98
o-xylene	hexadecane	-5.37
p-bromotoluene	hexadecane	-6.19
p-cresol	hexadecane	-5.88
pentanal	hexadecane	-3.89
pentanoic acid	hexadecane	-4.61
pentyl acetate	hexadecane	-5.20
pentylamine	hexadecane	-4.28
phenol	hexadecane	-5.14
propanal	hexadecane	-2.48
propanoic acid	hexadecane	-3.12
propene	hexadecane	-1.29
propionitrile	hexadecane	-2.84
propyl acetate	hexadecane	-3.93
propylamine	hexadecane	-2.92
propyne	hexadecane	-1.40
p-xylene	hexadecane	-5.24
pyridine	hexadecane	-4.10
s-trans-1,3-butadiene	hexadecane	-2.10
t-butanol	hexadecane	-2.74
tetrachloroethene	hexadecane	-4.88
tetrahydrofuran	hexadecane	-3.60
tetrahydropyran	hexadecane	-4.08
tetramethylsilane	hexadecane	-2.92
thiophene	hexadecane	-4.01
thiophenol	hexadecane	-5.61
toluene	hexadecane	-4.54
trichloroethene	hexadecane	-4.08
trimethylamine	hexadecane	-2.21
urea	hexadecane	-6.37
water	hexadecane	-0.35
benzene	hexadecyliodide	-3.71
chloroform	hexadecyliodide	-3.36
cyclohexane	hexadecyliodide	-3.66
dichloromethane	hexadecyliodide	-2.76
methylcyclohexane	hexadecyliodide	-4.07
n-heptane	hexadecyliodide	-3.90
n-hexane	hexadecyliodide	-3.26
n-pentane	hexadecyliodide	-2.59
toluene	hexadecyliodide	-4.41
1,4-dichlorobenzene	hexane	-5.69
1,4-dioxane	hexane	-4.08
1-butanol	hexane	-3.77
1-heptanol	hexane	-5.75
1-hexanol	hexane	-5.14
1-nitrobutane	hexane	-4.64
1-pentanol	hexane	-4.38
1-propanol	hexane	-2.81
2-butanone	hexane	-3.48
2-heptanone	hexane	-5.36
2-hexanone	hexane	-4.68
3,3-dimethylbutanone	hexane	-4.34
3,5-dibromo-4-hydroxybenzonitrile	hexane	-9.67
4-methylaniline	hexane	-6.18
acetic acid	hexane	-2.83
acetone	hexane	-2.60
acetophenone	hexane	-6.05

aniline	hexane	-5.43
benzaldehyde	hexane	-5.53
benzamide	hexane	-7.77
benzene	hexane	-3.96
bromobenzene	hexane	-5.66
bromoform	hexane	-4.38
butyl acetate	hexane	-4.86
butylamine	hexane	-3.62
chlorobenzene	hexane	-5.14
chloroform	hexane	-3.17
ethanol	hexane	-2.73
ethyl acetate	hexane	-3.62
ethylamine	hexane	-2.09
ethylbenzene	hexane	-4.99
fluorobenzene	hexane	-4.15
methanol	hexane	-1.49
methyl acetate	hexane	-3.12
methyl hexanoate	hexane	-5.64
methyl pentanoate	hexane	-4.94
methyl propanoate	hexane	-3.65
m-xylene	hexane	-4.99
n-hexane	hexane	-4.00
nitrobenzene	hexane	-6.09
nitroethane	hexane	-3.19
nitromethane	hexane	-2.90
n-octane	hexane	-5.46
o-cresol	hexane	-6.25
o-xylene	hexane	-5.22
p-bromophenol	hexane	-6.96
p-cresol	hexane	-5.86
pentyl acetate	hexane	-5.52
phenol	hexane	-5.49
p-hydroxybenzaldehyde	hexane	-9.18
propanoic acid	hexane	-2.98
propyl acetate	hexane	-4.10
propylamine	hexane	-3.13
p-xylene	hexane	-5.01
pyridine	hexane	-3.81
toluene	hexane	-4.84
triethylphosphate	hexane	-6.78
trimethylphosphate	hexane	-5.82
tripropylphosphate	hexane	-7.24
1-hexanol	hexanol	-7.05
acetic acid	hexanol	-6.51
benzene	hexanol	-3.68
butylamine	hexanol	-5.50
ethylamine	hexanol	-4.20
ethylbenzene	hexanol	-4.54
formaldehyde	hexanol	-3.42
m-cresol	hexanol	-8.42
o-cresol	hexanol	-8.76
p-bromophenol	hexanol	-10.51
p-cresol	hexanol	-9.21
phenol	hexanol	-8.76
propylamine	hexanol	-4.83
toluene	hexanol	-4.27
1,4-dioxane	iodobenzene	-4.94
1-butanol	iodobenzene	-4.05
1-heptanol	iodobenzene	-6.53
1-hexanol	iodobenzene	-5.71
1-pentanol	iodobenzene	-5.02
1-propanol	iodobenzene	-3.52
2-butanone	iodobenzene	-4.22
butylamine	iodobenzene	-4.19
ethanol	iodobenzene	-3.18
ethylamine	iodobenzene	-2.73
m-cresol	iodobenzene	-6.04
methanol	iodobenzene	-2.18
nitromethane	iodobenzene	-4.10
n-octane	iodobenzene	-4.72

o-cresol	iodobenzene	-6.76
o-cresol	iodobenzene	-7.14
p-bromophenol	iodobenzene	-8.45
p-cresol	iodobenzene	-7.01
propylamine	iodobenzene	-3.54
toluene	iodobenzene	-4.99
acetic acid	isobutanol	-6.80
butanal	isobutanol	-4.82
butanoic acid	isobutanol	-7.62
diethylamine	isobutanol	-4.86
dimethylamine	isobutanol	-4.43
dipropylamine	isobutanol	-5.87
ethyl acetate	isobutanol	-4.27
hexanoic acid	isobutanol	-8.77
hydrogen peroxide	isobutanol	-7.93
isobutanol	isobutanol	-5.79
methylamine	isobutanol	-4.56
pentanoic acid	isobutanol	-8.06
piperazine	isobutanol	-6.58
piperidine	isobutanol	-6.17
propanoic acid	isobutanol	-6.98
pyridine	isobutanol	-5.87
trimethylamine	isobutanol	-3.90
1,4-dioxane	isooctane	-4.02
1-butanol	isooctane	-3.56
1-butene	isooctane	-2.26
1-hexanol	isooctane	-5.10
1-nitropropane	isooctane	-3.94
1-pentanol	isooctane	-4.17
1-pentene	isooctane	-2.36
1-propanethiol	isooctane	-3.78
1-propanol	isooctane	-3.00
2-butanone	isooctane	-3.40
2-hexanone	isooctane	-4.72
2-pentanone	isooctane	-4.14
acetone	isooctane	-2.44
aniline	isooctane	-5.20
benzene	isooctane	-4.01
butanal	isooctane	-3.45
butylamine	isooctane	-3.57
chloroform	isooctane	-3.06
ethanethiol	isooctane	-3.13
ethanol	isooctane	-2.44
methyl benzoate	isooctane	-6.71
m-xylene	isooctane	-5.12
n-hexane	isooctane	-3.08
nitromethane	isooctane	-2.82
n-octane	isooctane	-5.44
n-pentane	isooctane	-3.21
o-cresol	isooctane	-5.68
p-cresol	isooctane	-5.59
pentanal	isooctane	-4.24
phenol	isooctane	-5.30
propene	isooctane	-1.61
toluene	isooctane	-4.68
1,4-dioxane	isopropanol	-4.49
2-butanone	isopropanol	-4.07
ethanol	isopropanol	-4.84
isopropanol	isopropanol	-4.82
nitromethane	isopropanol	-4.00
n-octane	isopropanol	-4.50
toluene	isopropanol	-4.38
2-butanone	isopropylbenzene	-4.02
2-heptanone	isopropylbenzene	-5.99
2-hexanone	isopropylbenzene	-5.39
2-pentanone	isopropylbenzene	-4.84
3,3-dimethylbutanone	isopropylbenzene	-4.81
acetone	isopropylbenzene	-3.32
butanoic acid	isopropylbenzene	-4.93
butyl acetate	isopropylbenzene	-5.36

butylamine	isopropylbenzene	-4.06
ethanol	isopropylbenzene	-2.90
ethyl acetate	isopropylbenzene	-4.22
isopropylbenzene	isopropylbenzene	-6.04
methyl hexanoate	isopropylbenzene	-6.19
methyl pentanoate	isopropylbenzene	-5.45
methyl propanoate	isopropylbenzene	-4.19
pentyl acetate	isopropylbenzene	-6.13
propanoic acid	isopropylbenzene	-4.23
propyl acetate	isopropylbenzene	-4.78
water	isopropylbenzene	-1.41
butylamine	isopropyltoluene	-4.22
methyl acetate	isopropyltoluene	-3.32
methyl hexanoate	isopropyltoluene	-6.06
methyl pentanoate	isopropyltoluene	-5.33
methyl propanoate	isopropyltoluene	-4.14
pentyl acetate	isopropyltoluene	-6.02
1,4-dioxane	mcresol	-6.82
2-butanone	mcresol	-5.98
ethanol	mcresol	-5.58
m-cresol	mcresol	-8.40
nitromethane	mcresol	-4.73
n-octane	mcresol	-4.02
toluene	mcresol	-4.58
2-butanone	mesitylene	-3.95
2-heptanone	mesitylene	-5.99
2-hexanone	mesitylene	-5.34
2-pentanone	mesitylene	-4.80
3,3-dimethylbutanone	mesitylene	-4.77
mesitylene	mesitylene	-6.40
phenol	mesitylene	-6.80
1,4-dioxane	methoxyethanol	-4.91
2-butanone	methoxyethanol	-4.28
ethanol	methoxyethanol	-4.71
nitromethane	methoxyethanol	-5.06
n-octane	methoxyethanol	-3.71
toluene	methoxyethanol	-4.49
1,4-dioxane	methylenechloride	-5.33
dichloromethane	methylenechloride	-3.80
ethanol	methylenechloride	-3.82
nitromethane	methylenechloride	-5.05
n-octane	methylenechloride	-5.18
p-bromophenol	methylenechloride	-9.09
p-cresol	methylenechloride	-7.71
phenol	methylenechloride	-7.50
thiophenol	methylenechloride	-7.11
toluene	methylenechloride	-5.53
water	methylenechloride	-2.63
1,4-dioxane	methylformamide	-4.86
2-butanone	methylformamide	-4.34
ethanol	methylformamide	-5.12
nitromethane	methylformamide	-5.11
N-methylformamide	methylformamide	-8.27
n-octane	methylformamide	-3.34
toluene	methylformamide	-4.34
acetic acid	nitrobenzene	-4.78
aniline	nitrobenzene	-7.15
butanoic acid	nitrobenzene	-5.84
hexanoic acid	nitrobenzene	-7.26
hydrogen peroxide	nitrobenzene	-5.45
m-cresol	nitrobenzene	-7.29
methanol	nitrobenzene	-2.93
nitrobenzene	nitrobenzene	-7.94
nitromethane	nitrobenzene	-4.90
o-cresol	nitrobenzene	-8.16
p-bromophenol	nitrobenzene	-9.76
p-cresol	nitrobenzene	-8.13
pentanoic acid	nitrobenzene	-6.47
phenol	nitrobenzene	-7.86
propanoic acid	nitrobenzene	-5.38

1,4-dioxane	nitroethane	-5.28
2-butanone	nitroethane	-4.73
ethanol	nitroethane	-3.98
nitroethane	nitroethane	-5.53
nitromethane	nitroethane	-5.35
n-octane	nitroethane	-3.89
toluene	nitroethane	-4.88
1,4-dioxane	nitromethane	-5.46
2-butanone	nitromethane	-4.72
ethanol	nitromethane	-4.16
g-butyrolactone	nitromethane	-5.45
nitromethane	nitromethane	-5.38
n-octane	nitromethane	-3.15
toluene	nitromethane	-4.52
1-butanol	nonane	-3.77
1-heptanol	nonane	-5.62
1-hexanol	nonane	-4.97
1-pentanol	nonane	-3.92
1-propanol	nonane	-2.76
2-butanone	nonane	-3.20
2-heptanone	nonane	-5.24
2-hexanone	nonane	-4.59
2-pentanone	nonane	-3.97
3,3-dimethylbutanone	nonane	-4.19
butyl acetate	nonane	-4.69
butylamine	nonane	-3.55
ethanol	nonane	-2.15
ethyl acetate	nonane	-3.45
ethylamine	nonane	-1.98
methanol	nonane	-1.29
methyl acetate	nonane	-3.02
methyl hexanoate	nonane	-5.51
methyl pentanoate	nonane	-4.85
methyl propanoate	nonane	-3.50
n-nonane	nonane	-5.91
o-cresol	nonane	-6.20
pentyl acetate	nonane	-5.33
phenol	nonane	-5.60
propyl acetate	nonane	-4.07
propylamine	nonane	-2.96
1-nonanol	nonanol	-9.05
2-methoxyethanol	nonanol	-5.61
benzene	nonanol	-3.82
butylamine	nonanol	-5.35
ethylamine	nonanol	-4.02
ethylbenzene	nonanol	-4.61
p-bromophenol	nonanol	-10.36
phenol	nonanol	-8.61
propylamine	nonanol	-4.66
toluene	nonanol	-4.34
1-butanol	octane	-3.69
1-heptanol	octane	-5.56
1-hexanol	octane	-4.86
1-nitropropane	octane	-3.95
1-pentanol	octane	-4.10
1-propanol	octane	-2.76
2-butanone	octane	-3.24
2-ethylpyrazine	octane	-5.51
2-heptanone	octane	-5.25
2-hexanone	octane	-4.60
2-methylaniline	octane	-6.06
2-methylpyrazine	octane	-4.70
2-pentanone	octane	-3.97
3,3-dimethylbutanone	octane	-4.21
3-methylaniline	octane	-6.15
4-methylaniline	octane	-6.00
acetone	octane	-2.46
aniline	octane	-4.84
butyl acetate	octane	-4.80
butylamine	octane	-3.44

diethylamine	octane	-3.42
ethanol	octane	-2.15
ethyl acetate	octane	-3.48
ethylamine	octane	-2.04
m-cresol	octane	-5.19
methanol	octane	-1.29
methyl acetate	octane	-3.06
methyl hexanoate	octane	-5.53
methyl pentanoate	octane	-4.86
methyl propanoate	octane	-3.57
n-octane	octane	-5.28
o-cresol	octane	-6.16
p-cresol	octane	-6.19
pentyl acetate	octane	-5.36
phenol	octane	-5.47
propyl acetate	octane	-4.09
propylamine	octane	-3.00
toluene	octane	-4.82
1,1,1,3,3,3-hexafluoropropan-2-ol	octanol	-5.76
1,1,1-trichloroethane	octanol	-3.69
1,1,1-trifluoropropan-2-ol	octanol	-5.12
1,1,2-trichloro-1,2,2-trifluoroethane	octanol	-2.54
1,1,2-trichloroethane	octanol	-4.53
1,1-dichloro-2,2-difluoroethyl methyl ether	octanol	-4.02
1,1-difluoroethane	octanol	-1.13
1,1-dimethyl-3-phenylurea	octanol	-13.12
1,2-dichlorobenzene	octanol	-6.01
1,2-dichloroethene	octanol	-3.61
1,2-dimethoxyethane	octanol	-4.55
1,2-ethanediol	octanol	-7.44
1,4-dichlorobenzene	octanol	-5.67
1,4-dioxane	octanol	-4.89
1-bromo-1-chloro-2,2,2-trifluoroethane	octanol	-3.27
1-bromobutane	octanol	-4.16
1-bromopentane	octanol	-4.68
1-bromopropane	octanol	-3.42
1-butanol	octanol	-5.71
1-butene	octanol	-1.89
1-chloropropane	octanol	-3.06
1-decanol	octanol	-9.88
1-heptanol	octanol	-7.75
1-hexanol	octanol	-7.06
1-hexene	octanol	-2.94
1-hexyne	octanol	-3.43
1-nitrobutane	octanol	-5.11
1-nitropropane	octanol	-4.44
1-octanol	octanol	-8.13
1-pentanol	octanol	-6.40
1-pentyne	octanol	-2.79
1-propanethiol	octanol	-3.52
1-propanol	octanol	-5.02
2,2,2-trifluoroethanol	octanol	-4.81
2,2',3'-trichlorobiphenyl	octanol	-9.12
2,2'-dichlorobiphenyl	octanol	-9.41
2,2-dichloroethenyl dimethyl phosphate	octanol	-8.59
2,2-dimethylpropane	octanol	-1.74
2,3-dichlorobiphenyl	octanol	-9.23
2,6-dichlorobenzonitrile	octanol	-9.18
2-bromopropane	octanol	-3.40
2-butanone	octanol	-3.78
2-chloropropane	octanol	-2.84
2-ethylpyrazine	octanol	-6.40
2-heptanone	octanol	-5.65
2-hexanone	octanol	-5.02
2-methoxyethanol	octanol	-5.83
2-methyl-1-nitrobenzene	octanol	-6.80
2-methylaniline	octanol	-7.36
2-methylpropane	octanol	-1.45
2-methylpropene	octanol	-2.03
2-methylpyrazine	octanol	-5.87

2-methylpyridine	octanol	-6.14
2-nitropropane	octanol	-4.23
2-octanone	octanol	-6.38
2-pentanone	octanol	-4.35
2-pyrrolidinone	octanol	-8.85
3,3-dimethylbutanone	octanol	-4.53
3-bromopropene	octanol	-3.30
3-ethyl-2-methoxypyrazine	octanol	-6.85
3-methylaniline	octanol	-7.57
3-methylpyridine	octanol	-6.40
3-pentanone	octanol	-4.36
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	octanol	-12.37
4-ethylpyridine	octanol	-7.80
4-methylaniline	octanol	-7.44
4-methylpyridine	octanol	-6.60
9-methyladenine	octanol	-13.56
acetic acid	octanol	-6.35
acetone	octanol	-3.15
acetonitrile	octanol	-3.15
acetophenone	octanol	-6.74
allyl alcohol	octanol	-5.27
aniline	octanol	-6.71
anisole	octanol	-5.47
anthracene	octanol	-10.47
benzaldehyde	octanol	-6.13
benzamide	octanol	-11.77
benzene	octanol	-3.72
benzonitrile	octanol	-6.09
bromobenzene	octanol	-5.46
bromoethane	octanol	-2.90
bromoform	octanol	-5.62
bromomethane	octanol	-2.43
bromotoluene	octanol	-6.36
bromotrifluoromethane	octanol	-0.75
butanal	octanol	-4.62
butanoic acid	octanol	-7.58
butanonitrile	octanol	-4.25
butyl acetate	octanol	-4.96
butylamine	octanol	-5.33
chlorobenzene	octanol	-5.00
chlorodifluoromethane	octanol	-1.97
chloroethane	octanol	-2.58
chloroform	octanol	-3.81
cyclohexane	octanol	-3.46
cyclopentane	octanol	-2.65
cyclopentanone	octanol	-5.01
cyclopropane	octanol	-1.60
dibromomethane	octanol	-4.18
dichloromethane	octanol	-3.07
diethyl 2,4-dichlorophenyl thiophosphate	octanol	-10.87
diethyl 4-nitrophenyl thiophosphonate	octanol	-11.31
diethyl ether	octanol	-2.89
diethyl sulfide	octanol	-4.09
diethylamine	octanol	-4.75
difluorodichloromethane	octanol	-1.25
dimethyl 2,4,5-trichlorophenyl thiophosphate	octanol	-11.69
dimethyl 4-bromo-2,5-dichlorophenyl thiophosphate	octanol	-12.30
dimethyl 4-nitrophenyl thiophosphate	octanol	-11.70
dimethyl disulfide	octanol	-4.24
dimethyl ether	octanol	-2.06
dipropylamine	octanol	-6.02
ethane	octanol	-0.64
ethanol	octanol	-4.36
ethene	octanol	-0.27
ethyl 4-cyanophenyl phenylthiophosphonate	octanol	-11.06
ethyl acetate	octanol	-4.06
ethyl phenyl ether	octanol	-5.65
ethylamine	octanol	-4.09
ethylbenzene	octanol	-5.08
ethyne	octanol	-0.51

fluorobenzene	octanol	-3.87
fluorotrichloromethane	octanol	-2.63
formaldehyde	octanol	-3.23
formamide	octanol	-7.80
g-butyrolactone	octanol	-6.83
hexanoic acid	octanol	-8.82
hydrazine	octanol	-3.44
hydrogen	octanol	1.76
isopropanol	octanol	-4.62
m-cresol	octanol	-8.20
methane	octanol	0.51
methanol	octanol	-3.87
methyl 3-methyl-4-thiomethoxyphenyl thiophosphate	octanol	-12.55
methyl acetate	octanol	-3.54
methyl benzoate	octanol	-7.26
methyl butanoate	octanol	-4.59
methyl formate	octanol	-2.82
methyl isopropyl ether	octanol	-4.64
methyl pentanoate	octanol	-5.13
methyl propanoate	octanol	-4.06
methyl propyl ether	octanol	-3.63
methylamine	octanol	-3.78
methylcyclohexane	octanol	-3.21
methylhydrazine	octanol	-3.88
m-hydroxybenzaldehyde	octanol	-11.39
morpholine	octanol	-5.99
m-xylene	octanol	-5.25
N,N-dimethylacetamide	octanol	-7.48
N,N-dimethylformamide	octanol	-6.14
naphthalene	octanol	-6.97
n-butane	octanol	-1.86
n-heptane	octanol	-3.74
n-hexane	octanol	-3.01
nitrobenzene	octanol	-6.63
nitroethane	octanol	-3.93
nitromethane	octanol	-3.51
N-methyl-2-pyrrolidinone	octanol	-8.63
N-methylaniline	octanol	-6.94
N-methylformamide	octanol	-6.97
n-octane	octanol	-4.18
n-pentane	octanol	-2.45
n-propane	octanol	-1.26
o-cresol	octanol	-8.49
O-ethyl O'-4-bromo-2-chlorophenyl S-propyl phosphorothioate	octanol	-10.49
o-xylene	octanol	-5.07
p-bromophenol	octanol	-10.59
p-cresol	octanol	-8.84
p-dibromobenzene	octanol	-7.47
pentanoic acid	octanol	-8.22
phenol	octanol	-8.69
p-hydroxybenzaldehyde	octanol	-12.36
piperazine	octanol	-5.80
piperidine	octanol	-6.27
propanal	octanol	-4.13
propanoic acid	octanol	-6.86
propene	octanol	-1.14
propionitrile	octanol	-3.66
propyl acetate	octanol	-4.55
propylamine	octanol	-4.77
propyne	octanol	-1.59
p-xylene	octanol	-5.19
pyridine	octanol	-5.34
pyrrole	octanol	-5.28
quinoline	octanol	-8.43
s-trans-1,3-butadiene	octanol	-2.10
t-butanol	octanol	-4.78
t-butyl methyl ether	octanol	-3.49
tetrachloroethene	octanol	-4.24
tetrafluoromethane	octanol	1.50
tetrahydrofuran	octanol	-3.93

tetrahydropyran	octanol	-4.21
tetramethylsilane	octanol	-1.79
thioanisole	octanol	-6.47
thiophene	octanol	-3.89
thiophenol	octanol	-5.99
toluene	octanol	-4.55
trichloroethene	octanol	-3.75
triethylphosphate	octanol	-8.88
trimethylamine	octanol	-3.60
trimethylphosphate	octanol	-7.81
tripropylphosphate	octanol	-8.65
urea	octanol	-10.93
water	octanol	-4.43
Z-1,2-dichloroethene	octanol	-3.71
1,2-dichlorobenzene	odichlorobenzene	-6.89
1-butanol	odichlorobenzene	-3.90
1-heptanol	odichlorobenzene	-6.50
1-hexanol	odichlorobenzene	-5.70
1-pentanol	odichlorobenzene	-4.93
1-propanol	odichlorobenzene	-3.47
butylamine	odichlorobenzene	-4.13
ethanol	odichlorobenzene	-2.34
ethylamine	odichlorobenzene	-2.59
methanol	odichlorobenzene	-1.73
propylamine	odichlorobenzene	-3.44
2-methyl-1-nitrobenzene	onitrotoluene	-8.04
acetic acid	onitrotoluene	-4.68
butanoic acid	onitrotoluene	-5.76
p-bromophenol	onitrotoluene	-9.57
phenol	onitrotoluene	-7.79
propanoic acid	onitrotoluene	-5.30
butyl acetate	pentadecane	-4.49
ethyl acetate	pentadecane	-3.37
methyl acetate	pentadecane	-2.82
methyl hexanoate	pentadecane	-5.35
methyl pentanoate	pentadecane	-4.59
methyl propanoate	pentadecane	-3.35
n-pentadecane	pentadecane	-9.91
pentyl acetate	pentadecane	-5.18
propyl acetate	pentadecane	-3.91
1-butanol	pentane	-3.77
1-heptanol	pentane	-5.62
1-hexanol	pentane	-4.97
1-pentanol	pentane	-3.92
1-propanol	pentane	-2.76
2-heptanone	pentane	-5.40
2-hexanone	pentane	-4.79
2-pentanone	pentane	-4.16
3,3-dimethylbutanone	pentane	-4.43
aniline	pentane	-5.15
bromoform	pentane	-4.83
butyl acetate	pentane	-4.88
chloroform	pentane	-3.26
ethanol	pentane	-2.15
ethyl acetate	pentane	-3.69
ethylamine	pentane	-2.18
methanol	pentane	-1.29
methyl acetate	pentane	-3.13
methyl hexanoate	pentane	-5.67
methyl pentanoate	pentane	-4.96
methyl propanoate	pentane	-3.69
n-pentane	pentane	-3.35
pentyl acetate	pentane	-5.62
phenol	pentane	-5.67
propyl acetate	pentane	-4.21
propylamine	pentane	-3.13
1-pentanol	pentanol	-7.92
acetic acid	pentanol	-6.65
ammonia	pentanol	-3.13
aniline	pentanol	-6.44

benzene	pentanol	-3.53
butanoic acid	pentanol	-7.74
butylamine	pentanol	-5.55
diethylamine	pentanol	-5.30
ethylamine	pentanol	-4.27
ethylbenzene	pentanol	-4.48
formaldehyde	pentanol	-3.44
hexanoic acid	pentanol	-8.99
hydrogen peroxide	pentanol	-7.46
methylamine	pentanol	-3.95
o-cresol	pentanol	-8.57
p-bromophenol	pentanol	-10.62
p-cresol	pentanol	-9.25
pentanoic acid	pentanol	-8.17
phenol	pentanol	-8.55
propanoic acid	pentanol	-7.09
propylamine	pentanol	-4.88
toluene	pentanol	-4.25
2-heptanone	perfluorobenzene	-6.15
2-hexanone	perfluorobenzene	-5.55
2-pentanone	perfluorobenzene	-5.10
3,3-dimethylbutanone	perfluorobenzene	-5.26
acetone	perfluorobenzene	-3.82
butyl acetate	perfluorobenzene	-5.52
butylamine	perfluorobenzene	-4.13
ethyl acetate	perfluorobenzene	-4.56
methyl acetate	perfluorobenzene	-4.23
methyl hexanoate	perfluorobenzene	-6.21
methyl pentanoate	perfluorobenzene	-5.59
nitromethane	perfluorobenzene	-4.30
pentyl acetate	perfluorobenzene	-6.16
perfluorobenzene	perfluorobenzene	-4.42
propyl acetate	perfluorobenzene	-5.06
1,4-dioxane	phenylether	-4.83
2-butanone	phenylether	-4.08
ethanol	phenylether	-3.22
nitromethane	phenylether	-4.19
n-octane	phenylether	-4.38
toluene	phenylether	-4.86
1,4-dioxane	propanol	-4.61
1-propanol	propanol	-5.29
2-butanone	propanol	-4.15
ethanol	propanol	-5.01
nitromethane	propanol	-4.04
n-octane	propanol	-4.39
toluene	propanol	-4.47
1,4-dioxane	pyridine	-5.14
2-butanone	pyridine	-4.61
ethanol	pyridine	-5.08
nitromethane	pyridine	-5.11
n-octane	pyridine	-4.50
pyridine	pyridine	-5.47
toluene	pyridine	-5.10
acetic acid	secbutanol	-6.81
butanoic acid	secbutanol	-7.34
butylamine	secbutanol	-5.52
formaldehyde	secbutanol	-2.86
hexanoic acid	secbutanol	-8.11
pentanoic acid	secbutanol	-7.61
propanoic acid	secbutanol	-7.00
secbutanol	secbutanol	-5.48
water	secbutanol	-5.71
butyl acetate	secbutylbenzene	-5.22
ethyl acetate	secbutylbenzene	-4.11
methyl acetate	secbutylbenzene	-3.91
pentyl acetate	secbutylbenzene	-5.98
propyl acetate	secbutylbenzene	-4.62
2-butanone	tbutylbenzene	-3.94
2-heptanone	tbutylbenzene	-5.88
2-hexanone	tbutylbenzene	-5.27

2-pentanone	tbutylbenzene	-4.72
3,3-dimethylbutanone	tbutylbenzene	-4.79
butyl acetate	tbutylbenzene	-5.25
ethyl acetate	tbutylbenzene	-4.22
methyl acetate	tbutylbenzene	-3.57
methyl hexanoate	tbutylbenzene	-6.13
methyl pentanoate	tbutylbenzene	-5.39
methyl propanoate	tbutylbenzene	-4.17
pentyl acetate	tbutylbenzene	-5.92
propyl acetate	tbutylbenzene	-4.72
tbutylbenzene	tbutylbenzene	-6.43
acetone	tetrachloroethene	-3.09
butyl acetate	tetrachloroethene	-5.35
butylamine	tetrachloroethene	-4.49
ethyl acetate	tetrachloroethene	-4.22
methyl acetate	tetrachloroethene	-3.63
methyl pentanoate	tetrachloroethene	-5.41
methyl propanoate	tetrachloroethene	-4.39
phenol	tetrachloroethene	-6.10
propyl acetate	tetrachloroethene	-4.80
tetrachloroethene	tetrachloroethene	-5.39
1,4-dioxane	tetrahydrofuran	-5.17
2-butanone	tetrahydrofuran	-4.54
ethanol	tetrahydrofuran	-4.56
nitromethane	tetrahydrofuran	-5.09
n-octane	tetrahydrofuran	-5.39
tetrahydrofuran	tetrahydrofuran	-4.25
toluene	tetrahydrofuran	-5.50
1,4-dioxane	tetrahydrothiophenedioxide	-4.90
2-butanone	tetrahydrothiophenedioxide	-4.09
butylamine	tetrahydrothiophenedioxide	-4.25
ethanol	tetrahydrothiophenedioxide	-4.30
nitromethane	tetrahydrothiophenedioxide	-5.28
n-octane	tetrahydrothiophenedioxide	-2.44
toluene	tetrahydrothiophenedioxide	-4.23
2-butanone	tetralin	-3.12
2-heptanone	tetralin	-5.33
2-hexanone	tetralin	-4.64
2-pentanone	tetralin	-3.99
3,3-dimethylbutanone	tetralin	-4.19
acetone	tetralin	-2.54
ethanol	tetralin	-1.54
tetralin	tetralin	-7.55
water	tetralin	0.07
1,4-dioxane	toluene	-4.91
1-butanol	toluene	-4.31
1-heptanol	toluene	-6.75
1-hexanol	toluene	-6.12
1-nitropropane	toluene	-5.25
1-pentanol	toluene	-5.17
1-propanol	toluene	-3.71
2-butanone	toluene	-4.27
2-heptanone	toluene	-6.30
2-hexanone	toluene	-5.60
2-pentanone	toluene	-5.02
3,3-dimethylbutanone	toluene	-5.00
4-methylaniline	toluene	-7.39
acetic acid	toluene	-4.00
acetone	toluene	-3.59
ammonia	toluene	-2.38
aniline	toluene	-6.69
butanoic acid	toluene	-5.24
butyl acetate	toluene	-5.57
butylamine	toluene	-4.33
diethylamine	toluene	-3.75
dimethylamine	toluene	-2.68
dipropylamine	toluene	-5.24
ethanol	toluene	-3.33
ethyl acetate	toluene	-4.41
ethylamine	toluene	-2.67

g-butyrolactone	toluene	-4.70
hexanoic acid	toluene	-6.97
hydrogen peroxide	toluene	-3.14
methanol	toluene	-2.18
methyl acetate	toluene	-3.81
methyl benzoate	toluene	-7.96
methyl hexanoate	toluene	-6.38
methyl pentanoate	toluene	-5.65
methyl propanoate	toluene	-4.62
methylamine	toluene	-2.65
nitromethane	toluene	-4.31
n-octane	toluene	-5.38
o-cresol	toluene	-7.43
p-bromophenol	toluene	-8.70
p-cresol	toluene	-7.56
pentanoic acid	toluene	-5.89
pentyl acetate	toluene	-6.41
phenol	toluene	-6.93
propanoic acid	toluene	-4.57
propyl acetate	toluene	-5.00
propylamine	toluene	-3.51
pyridine	toluene	-5.13
toluene	toluene	-5.12
trimethylamine	toluene	-2.71
water	toluene	-1.69
1-butanol	tributylphosphate	-6.28
1-heptanol	tributylphosphate	-7.98
1-hexanol	tributylphosphate	-7.68
1-pentanol	tributylphosphate	-6.69
1-propanol	tributylphosphate	-5.42
2-methoxyethanol	tributylphosphate	-6.14
acetic acid	tributylphosphate	-7.11
aniline	tributylphosphate	-7.60
butanoic acid	tributylphosphate	-8.29
ethanol	tributylphosphate	-4.57
ethylamine	tributylphosphate	-3.29
methanol	tributylphosphate	-4.16
pentanoic acid	tributylphosphate	-8.82
propanoic acid	tributylphosphate	-7.73
propylamine	tributylphosphate	-3.98
water	tributylphosphate	-4.69
1,4-dioxane	triethylamine	-4.41
2-butanone	triethylamine	-3.86
ethanol	triethylamine	-4.02
nitromethane	triethylamine	-3.63
n-octane	triethylamine	-5.62
toluene	triethylamine	-4.98
triethylamine	triethylamine	-4.44
2-butanone	trimethylbenzene	-3.97
2-heptanone	trimethylbenzene	-6.01
2-hexanone	trimethylbenzene	-5.39
2-pentanone	trimethylbenzene	-4.83
3,3-dimethylbutanone	trimethylbenzene	-4.80
methyl acetate	trimethylbenzene	-3.58
methyl hexanoate	trimethylbenzene	-6.16
methyl pentanoate	trimethylbenzene	-5.41
methyl propanoate	trimethylbenzene	-4.14
pentyl acetate	trimethylbenzene	-6.09
trimethylbenzene	trimethylbenzene	-6.47
1,1,1-trichloroethane	undecane	-3.82
1,2-dichlorobenzene	undecane	-6.11
1,2-dichloroethene	undecane	-3.60
benzene	undecane	-4.05
bromoform	undecane	-4.84
butylamine	undecane	-3.55
chlorobenzene	undecane	-5.12
chloroform	undecane	-3.42
ethylbenzene	undecane	-5.44
n-undecane	undecane	-7.22
tetrachloroethene	undecane	-4.63

toluene	undecane	-4.81
trichloroethene	undecane	-3.87
1,4-dioxane	xylene	-4.86
1-butanol	xylene	-4.17
1-heptanol	xylene	-6.74
1-hexanol	xylene	-5.85
1-pentanol	xylene	-4.72
1-propanol	xylene	-3.57
2-butanone	xylene	-4.23
2-heptanone	xylene	-6.15
2-hexanone	xylene	-5.49
2-pentanone	xylene	-4.87
3,3-dimethylbutanone	xylene	-4.91
4-methylaniline	xylene	-7.17
acetic acid	xylene	-4.08
acetone	xylene	-3.26
aniline	xylene	-6.10
butanoic acid	xylene	-5.30
butyl acetate	xylene	-5.40
diethylamine	xylene	-3.93
dimethylamine	xylene	-3.36
dipropylamine	xylene	-5.35
ethanol	xylene	-3.42
ethyl acetate	xylene	-4.26
ethylamine	xylene	-3.01
hexanoic acid	xylene	-6.67
m-cresol	xylene	-6.32
methanol	xylene	-1.73
methyl acetate	xylene	-3.70
methyl hexanoate	xylene	-6.26
methyl pentanoate	xylene	-5.61
methyl propanoate	xylene	-4.20
methylamine	xylene	-3.20
nitromethane	xylene	-4.20
n-octane	xylene	-5.29
o-cresol	xylene	-7.25
p-bromophenol	xylene	-8.69
p-cresol	xylene	-7.18
pentanoic acid	xylene	-5.71
pentyl acetate	xylene	-6.19
pentylamine	xylene	-4.70
phenol	xylene	-6.83
piperidine	xylene	-5.15
propanoic acid	xylene	-4.72
propyl acetate	xylene	-4.87
propylamine	xylene	-3.69
pyridine	xylene	-5.12
toluene	xylene	-5.06
trimethylamine	xylene	-2.63
water	xylene	-1.56

20 nonaqueous data for 9 iodine-containing hydrocarbons from Zhu et. al., *J. Chem. Phys*. **1998**, *109*, 9117:

solute	**solvent keyword**	**free energy of solvation**
iodobenzene	carbontet	-6.50
iodobenzene	chloroform	-6.60
iodobenzene	cyclohexane	-6.26
iodobenzene	decalin	-5.96
iodobenzene	diethylether	-6.64
iodomethane	diethylether	-3.51
iodobenzene	heptane	-6.27
1-iodobutane	hexadecane	-4.95
1-iodopentane	hexadecane	-5.63
1-iodopropane	hexadecane	-4.27
3-iodopropene	hexadecane	-4.10
diiodomethane	hexadecane	-5.26
iodobenzene	hexadecane	-6.25
iodoethane	hexadecane	-3.51
iodomethane	hexadecane	-2.88
2-iodopropane	octanol	-4.40

diiodomethane	octanol	-5.63
iodobenzene	octanol	-6.18
iodoethane	octanol	-3.45
iodomethane	octanol	-3.07

17 nonaqueous data for five uracils taken from the SAMPL2 set of compounds:

solute	**solvent keyword**	**free energy of solvation**
uracil	butanol	-16.05
5-bromouracil	chloroform	-15.03
5-fluorouracil	chloroform	-14.31
uracil	chloroform	-14.28
5-bromouracil	diethylether	-17.01
5-fluorouracil	diethylether	-15.56
uracil	diethylether	-15.03
5-bromouracil	ethylacetate	-17.93
5-fluorouracil	ethylacetate	-16.10
uracil	ethylacetate	-15.43
5-bromouracil	heptane	-12.73
5-fluorouracil	heptane	-11.28
5-bromouracil	octanol	-17.88
5-chlorouracil	octanol	-17.26
5-fluorouracil	octanol	-15.71
5-trifluoromethyluracil	octanol	-15.51
uracil	octanol	-15.13

20 nonaqueous data for hexachlorocyclohexane (lindane) and for 19 SAMPL2 compounds:

solute	**solvent keyword**	**free energy of solvation**
1,2,3,4,5,6-hexachlorocyclohexane (lindane)	octanol	-10.71
acetylsalicylic acid	octanol	-11.56
butylparaben	octanol	-13.59
caffeine	octanol	-12.54
cyanuric acid	octanol	-18.89
diflunisal	octanol	-15.46
ethylparaben	octanol	-12.57
flurbiprofen (racemic)	octanol	-14.10
hexachlorobenzene	octanol	-10.15
ibuprofen (racemic)	octanol	-12.42
5-iodouracil	octanol	-18.77
ketoprofen (racemic)	octanol	-15.04
methylparaben	octanol	-12.18
naproxen	octanol	-14.55
4-nitroaniline	octanol	-11.35
octafluorocyclobutane	octanol	0.31
pentachloronitrobenzene	octanol	-11.55
phthalimide	octanol	-11.18
propylparaben	octanol	-13.52
sulfolane	octanol	-7.56

Table S6. 144 Reference Transfer Free Energies (kcal/mol) for 106 Neutral Solutes between Water and 14 Organic Solvents

126 transfer data taken from the SM8/SMD/SM8AD training set:

solute	solvent-water	transfer free energy
5-methyluracil (thymine)	benzene-water	1.77
acetanilide	benzene-water	-0.30
b-propiolactone	benzene-water	0.27
isopropyl methylphosphonofluoridate	benzene-water	-0.44
b-propiolactone	carbontet-water	-0.10
isopropyl methylphosphonofluoridate	carbontet-water	0.11
isopropyl methylphosphonofluoridate	chlorobenzene-water	-0.40
4-methyl-g-butyrolactone	chloroform-water	-1.29
acetanilide	chloroform-water	-1.20
b-propiolactone	chloroform-water	0.67
chloroacetamide	chloroform-water	1.31
isopropyl methylphosphonofluoridate	chloroform-water	-2.03
phenylurea	chloroform-water	0.86
trichloroacetamide	chloroform-water	-0.42
4-methyl-g-butyrolactone	cyclohexane-water	2.37
acetanilide	cyclohexane-water	1.92
isoquinoline	cyclohexane-water	-1.51
N,N-diethylacetamide	cyclohexane-water	1.93
trifluoroacetamide	cyclohexane-water	5.36
isopropyl methylphosphonofluoridate	dibromoethane-water	-0.48
5-methyluracil (thymine)	dibutylether-water	1.77
a-hydroxy-b,b-dimethylbutyrolactone	dichloroethane-water	0.80
b-propiolactone	dichloroethane-water	0.53
isopropyl methylphosphonofluoridate	dichloroethane-water	-1.70
5-methyluracil (thymine)	diethylether-water	1.43
acetanilide	diethylether-water	-0.74
b-propiolactone	diethylether-water	-0.03
chloroacetamide	diethylether-water	1.40
ethylurea	diethylether-water	3.25
methylurea	diethylether-water	3.97
phenylurea	diethylether-water	0.15
trichloroacetamide	diethylether-water	-1.47
5-methyluracil (thymine)	ethylacetate-water	1.01
acetanilide	heptane-water	1.80
isopropyl methylphosphonofluoridate	heptane-water	0.95
isoquinoline	heptane-water	-1.38
N,N-diethylacetamide	heptane-water	2.05
phenylurea	heptane-water	4.31
trichloroacetamide	heptane-water	1.21
acetanilide	hexane-water	1.35
isopropyl methylphosphonofluoridate	nitrobenzene-water	-0.55
1,1-dimethyl-3-(3-fluoro-phenyl)urea	octanol-water	-1.87
1,1-dimethyl-3-(4-bromo-phenyl)urea	octanol-water	-2.99
1,1-dimethyl-3-(4-fluoro-phenyl)urea	octanol-water	-1.54
1,2-benzodithiol-3-one	octanol-water	-3.72
1,2-benzodithiole-3-thione	octanol-water	-4.87
1,2-dithiol-3-one	octanol-water	-1.13
1,2-dithiol-3-thione	octanol-water	-2.25
1-ethyl-5-methyluracil	octanol-water	0.20
1-methyluracil	octanol-water	1.36
2,5-dimethylpyrrole	octanol-water	-2.00
2,6-difluoro acetanilide	octanol-water	-0.94
2-cyanopyrrole	octanol-water	-1.54
2-piperidinone	octanol-water	0.63
3-bromophenylurea	octanol-water	-2.84
3-chlorophenylyrea	octanol-water	-2.48
3-fluoroacetanilide	octanol-water	-2.14
3-fluorophenylurea	octanol-water	-1.76
3-methylacetanilide	octanol-water	-2.14
3-methylphenylurea	octanol-water	-1.75
3-methylthiophenylurea	octanol-water	-2.14
3-trifluoromethyl acetanilide	octanol-water	-3.25

3-trifluoromethylphenylurea	octanol-water	-3.15
4-(2-hydroxyethyl)pyridine	octanol-water	-0.14
4-(hydroxymethyl)pyridine	octanol-water	-0.08
4,5-dimethyl-1,2-dithiol-3-one	octanol-water	-2.36
4,5-dimethyl-1,2-dithiol-3-thione	octanol-water	-3.34
4-aminopyridine	octanol-water	-0.41
4-bromoacetanilide	octanol-water	-2.88
4-bromophenylurea	octanol-water	-2.70
4-bromopyridine	octanol-water	-2.10
4-chlorophenylurea	octanol-water	-2.45
4-fluoroacetanilide	octanol-water	-1.88
4-fluorophenylurea	octanol-water	-1.42
4-methyl-1,2-dithiol-3-one	octanol-water	-1.81
4-methyl-1,2-dithiol-3-thione	octanol-water	-2.97
4-methyl-5-phenyl-1,2-dithiol-3-thione	octanol-water	-5.39
4-methylacetanilide	octanol-water	-2.14
4-methyl-g-butyrolactone	octanol-water	0.48
4-nitropyridine	octanol-water	-0.45
4-phenyl-1,2-dithiol-3-one	octanol-water	-3.60
4-phenyl-1,2-dithiol-3-thione	octanol-water	-4.36
4-trimethylsilylphenol	octanol-water	-5.22
5-cyanouracil	octanol-water	1.26
5-methyl-1,2-dithiol-3-one	octanol-water	-1.72
5-methyl-1,2-dithiol-3-thione	octanol-water	-2.55
5-methyl-4-phenyl-1,2-dithiol-3-one	octanol-water	-4.00
5-methyl-4-phenyl-1,2-dithiol-3-thione	octanol-water	-4.32
5-methyluracil (thymine)	octanol-water	0.84
5-phenyl-1,2-dithiol-3-one	octanol-water	-4.11
5-phenyl-1,2-dithiol-3-thione	octanol-water	-5.01
acetanilide	octanol-water	-1.58
benzyltrimethylsilane	octanol-water	-5.62
bromoacetamide	octanol-water	0.71
butyldimethylsilane	octanol-water	-4.86
butyltrimethylsilane	octanol-water	-5.71
chloroacetamide	octanol-water	0.72
decamethyltetrasiloxane	octanol-water	-7.34
dimethylphenylphosphine	octanol-water	-3.50
dimethylphenylsilane	octanol-water	-5.43
dimethylpropylsilane	octanol-water	-4.38
diphenyldiethoxysilane	octanol-water	-6.69
ethylurea	octanol-water	1.01
fluoroacetamide	octanol-water	1.43
g-decalactone	octanol-water	-3.70
hexamethyldisiloxane	octanol-water	-5.71
isoquinoline	octanol-water	-2.84
methylurea	octanol-water	1.90
N-(tetrahydro-2-oxo-3-thienyl)acetamide	octanol-water	0.48
N,N-diethylacetamide	octanol-water	-0.46
N-benzyl-2-pyrrolidinone	octanol-water	-1.70
n-butylurea	octanol-water	-0.56
N-ethylcaprolactam	octanol-water	-0.88
N-methylpyrrole	octanol-water	-1.65
N-phenylpyrrole	octanol-water	-4.20
N-vinyl-2-pyrrolidinone	octanol-water	-0.50
octamethyltrisiloxane	octanol-water	-6.53
p-cyanoacetanilide	octanol-water	-1.87
phenylacetamide	octanol-water	-0.61
phenyltrimethylsilane	octanol-water	-6.42
phenylurea	octanol-water	-1.13
propyltrimethylsilane	octanol-water	-5.22
tetramethylurea	octanol-water	-0.26
trichloroacetamide	octanol-water	-1.41
triethoxyphenylsilane	octanol-water	-4.07
trifluoroacetamide	octanol-water	-0.16

18 transfer data taken from the PhysProp database:

solute	**solvent-water**	**transfer free energy**
2-fluoroanisole	octanol-water	-2.92

3-fluoroanisole	octanol-water	-3.22
4-fluoroanisole	octanol-water	-3.08
2-chloroanisole	octanol-water	-3.66
3-chloroanisole	octanol-water	-4.07
4-chloroanisole	octanol-water	-3.79
pentachloroanisole	octanol-water	-7.43
2-bromoanisole	octanol-water	-3.90
3-bromoanisole	octanol-water	-4.41
4-bromoanisole	octanol-water	-4.30
2,6-difluoropyridine	octanol-water	-1.60
cinnoline	octanol-water	-1.27
4-cyanopyridine	octanol-water	-0.63
4-acetylpyridine	octanol-water	-0.65
methyl phenyl sulfoxide	octanol-water	-0.75
methyl phenyl sulfone	octanol-water	-0.68
biphenyl	octanol-water	-5.43
9H-fluorene	octanol-water	-5.70

Table S7. Reference Solvation Free Energies (kcal/mol) for 112 Selectively Clustered Ions in Water

solute	charge	free energy of solvation
1-aminonaphthalene	+1	-67.4
2-methylaniline	+1	-70.3
3-aminoaniline	+1	-65.8
3-chloroaniline	+1	-74.7
3-methylaniline	+1	-69.6
4-chloroaniline	+1	-74.1
4-methoxyaniline	+1	-71.2
4-methylaniline	+1	-69.8
4-methyl-N,N-dimethylaniline	+1	-55.9
4-nitroaniline	+1	-75.9
acetamide	+1	-73.9
acetone (cluster)	+1	-66.3
acetonitrile	+1	-75.3
acetophenone (cluster)	+1	-55.7
allylamine	+1	-72.0
ammonia (cluster)	+1	-74.6
aniline	+1	-72.4
azacycloheptane	+1	-63.3
azetidine	+1	-67.7
aziridine	+1	-70.9
benzamide	+1	-67.2
cyclohexanamine	+1	-68.7
diallylamine	+1	-61.6
diethyl ether (cluster)	+1	-62.2
diethylamine	+1	-63.4
dimethyl ether (cluster)	+1	-66.3
dimethyl sulfide	+1	-64.5
dimethyl sulfoxide	+1	-67.7
dimethylamine	+1	-68.6
di-n-propylamine	+1	-60.5
ethanol (cluster)	+1	-73.6
hydrazine	+1	-84.6
isopropylamine	+1	-69.6
methanol (cluster)	+1	-76.6
methylamine	+1	-76.4
morpholine	+1	-69.6
N,N-diethylaniline	+1	-54.0
N,N-dimethylaniline	+1	-57.2
N-ethylaniline	+1	-62.2
N-methylaniline	+1	-62.6
n-propylamine	+1	-71.5
piperazine	+1	-66.0
piperidine	+1	-64.2
pyridine	+1	-61.1
pyrrole	+1	-61.4
pyrrolidine	+1	-66.0
quinoline	+1	-56.0
tert-butylamine	+1	-67.3
triethylamine	+1	-54.6
trimethylamine	+1	-61.1
tri-n-propylamine	+1	-50.9
water (cluster)	+1	-87.8
1,1,1,3,3,3-hexafluoropropan-2-ol (cluster)	-1	-61.6
1,2-ethanediol (cluster)	-1	-73.3
1-propanethiol	-1	-70.5
1-propanol (cluster)	-1	-75.8
2,2,2-trifluoroethanol (cluster)	-1	-68.0
2-butanol (cluster)	-1	-76.3
2-chlorophenol	-1	-66.1
2-methoxyethanol (cluster)	-1	-77.9
2-methylphenol	-1	-70.2
2-nitrophenol	-1	-60.1
3-hydroxyphenol	-1	-73.8

3-methylphenol	-1	-71.1
3-nitrophenol	-1	-61.9
3-pentanone	-1	-73.7
4-chlorophenol	-1	-66.0
4-hydroxyphenol	-1	-77.6
4-methylphenol	-1	-72.0
4-nitroaniline	-1	-57.4
4-nitrophenol	-1	-57.8
acetaldehyde	-1	-76.5
acetamide	-1	-80.2
acetic acid	-1	-77.6
acetone	-1	-76.2
acetonitrile	-1	-66.6
acetylene (cluster)	-1	-67.9
acrylic acid	-1	-74.0
allyl alcohol (cluster)	-1	-75.1
aniline	-1	-62.9
benzoic acid	-1	-71.2
benzyl alcohol (cluster)	-1	-75.4
chloroacetic acid	-1	-69.7
chloroform	-1	-54.1
cyanamide	-1	-72.2
dichloroacetic acid	-1	-62.3
dimethyl sulfoxide	-1	-67.7
diphenylamine	-1	-54.6
ethanethiol	-1	-71.8
ethanol (cluster)	-1	-78.5
ethyl hydroperoxide (cluster)	-1	-77.1
formic acid	-1	-76.2
hexanoic acid	-1	-74.6
hydrobromic acid (cluster)	-1	-63.2
hydrochloric acid (cluster)	-1	-67.5
hydrofluoric acid (cluster)	-1	-85.5
hydrogen cyanide (cluster)	-1	-64.0
hydrogen peroxide (cluster)	-1	-82.3
hydrogen sulfide (cluster)	-1	-65.5
hydroperoxyl radical (cluster)	-1	-73.2
isopropanol (cluster)	-1	-76.0
methanethiol	-1	-73.8
methanol (cluster)	-1	-80.1
methyl hydroperoxide (cluster)	-1	-80.6
nitromethane	-1	-76.5
phenol	-1	-71.9
propanoic acid	-1	-76.2
pyruvic acid	-1	-68.5
t-butanol (cluster)	-1	-72.1
thiophenol	-1	-63.4
trifluoroacetic acid	-1	-59.3
water (cluster)	-1	-86.9

Table S8. 220 Reference Solvation Free Energies (kcal/mol) for 166 Unclustered Ions in Acetonitrile, DMSO, and Methanol

solute	charge	solvent keyword	free energy of solvation
2,4-dimethylpyridine	+1	acetonitrile	-61.9
4-methylaniline	+1	acetonitrile	-74.4
4-methylbenzoic acid	+1	acetonitrile	-75.4
acetic acid	+1	acetonitrile	-85.9
acetone	+1	acetonitrile	-77.5
acetophenone	+1	acetonitrile	-69.2
ammonia	+1	acetonitrile	-89.3
aniline	+1	acetonitrile	-76.8
benzamide	+1	acetonitrile	-69.7
benzoic acid	+1	acetonitrile	-78.3
benzylamine	+1	acetonitrile	-78.2
diethyl ether	+1	acetonitrile	-71.0
diethylamine	+1	acetonitrile	-67.5
diisobutylamine	+1	acetonitrile	-65.4
dimethyl sulfoxide	+1	acetonitrile	-73.5
di-n-butylamine	+1	acetonitrile	-64.8
ethylamine	+1	acetonitrile	-76.8
hydrazine	+1	acetonitrile	-87.7
hydrogen sulfide	+1	acetonitrile	-100.2
isobutylamine	+1	acetonitrile	-73.5
methanol	+1	acetonitrile	-92.1
methoxybenzene	+1	acetonitrile	-70.4
methylamine	+1	acetonitrile	-80.2
morpholine	+1	acetonitrile	-74.1
n-butanol	+1	acetonitrile	-85.2
n-butylamine	+1	acetonitrile	-75.7
n-propylamine	+1	acetonitrile	-75.7
phenol	+1	acetonitrile	-78.1
piperidine	+1	acetonitrile	-69.2
pyridine	+1	acetonitrile	-66.7
pyrrolidine	+1	acetonitrile	-71.0
t-butanol	+1	acetonitrile	-82.4
t-butylamine	+1	acetonitrile	-70.9
tetrahydrofuran	+1	acetonitrile	-74.7
thioacetamide	+1	acetonitrile	-73.6
triethylamine	+1	acetonitrile	-59.8
trimethylamine	+1	acetonitrile	-66.1
tri-n-butylamine	+1	acetonitrile	-57.4
tri-n-propylamine	+1	acetonitrile	-57.9
2,4,6-trimethylbenzoic acid	-1	acetonitrile	-54.4
2,4-dinitrophenol	-1	acetonitrile	-36.0
2-chlorobenzoic acid	-1	acetonitrile	-53.5
2-hydroxybenzoic acid	-1	acetonitrile	-46.5
2-nitrobenzoic acid	-1	acetonitrile	-51.9
3,4,5-trichlorophenol	-1	acetonitrile	-43.8
3,4-dimethylbenzoic acid	-1	acetonitrile	-59.7
3-chlorophenol	-1	acetonitrile	-50.6
3-nitrobenzoic acid	-1	acetonitrile	-48.3
3-nitrophenol	-1	acetonitrile	-46.7
3-trifluoromethylphenol	-1	acetonitrile	-46.9
4-cyanophenol	-1	acetonitrile	-46.5
4-hydroxybenzoic acid	-1	acetonitrile	-53.8
4-nitrobenzoic acid	-1	acetonitrile	-48.0
4-nitrophenol	-1	acetonitrile	-45.0
acetic acid	-1	acetonitrile	-58.8
benzenesulfonamide	-1	acetonitrile	-55.4
benzoic acid	-1	acetonitrile	-55.4
butanoic acid	-1	acetonitrile	-56.7
chloroacetic acid	-1	acetonitrile	-54.6
cyanoacetic acid	-1	acetonitrile	-50.8
cyclohexanecarboxylic acid	-1	acetonitrile	-55.6
dichloroacetic acid	-1	acetonitrile	-51.2
glycolic acid	-1	acetonitrile	-54.7

hydrobromic acid	-1	acetonitrile	-59.3
hydrochloric acid	-1	acetonitrile	-62.4
methanesulfonic acid	-1	acetonitrile	-54.0
nitric acid	-1	acetonitrile	-51.0
phenol	-1	acetonitrile	-55.1
trifluoroacetic acid	-1	acetonitrile	-45.6
ammonia	+1	DMSO	-93.9
aniline	+1	DMSO	-79.8
methylamine	+1	DMSO	-82.4
pyridine	+1	DMSO	-67.2
1,2,3-triazole	-1	DMSO	-56.7
1,2,4-triazole	-1	DMSO	-57.2
2,2,2-trifluoroethanol	-1	DMSO	-56.1
2,4-dinitrophenol	-1	DMSO	-38.0
2-chlorobenzoic acid	-1	DMSO	-53.6
2-indanone	-1	DMSO	-58.7
2-methoxyacetamide	-1	DMSO	-59.5
2-naphthol	-1	DMSO	-51.8
2-nitrobenzoic acid	-1	DMSO	-52.6
2-nitropropane	-1	DMSO	-59.9
3,4-dimethylbenzoic acid	-1	DMSO	-59.8
3-aminobenzoic acid	-1	DMSO	-59.5
3-aminopyridine	-1	DMSO	-51.5
3-hydroxybenzoic acid	-1	DMSO	-56.5
3-methylbenzoic acid	-1	DMSO	-56.1
3-pentanone	-1	DMSO	-59.0
4-aminopyridine	-1	DMSO	-51.3
4-chlorobenzoic acid	-1	DMSO	-52.6
4-nitroaniline	-1	DMSO	-47.4
4-nitrobenzoic acid	-1	DMSO	-48.2
4-nitrophenol	-1	DMSO	-45.4
acetamide	-1	DMSO	-58.0
acetic acid	-1	DMSO	-59.2
acetone	-1	DMSO	-60.4
acetonitrile	-1	DMSO	-54.9
adenine	-1	DMSO	-56.4
aniline	-1	DMSO	-52.9
benzamide	-1	DMSO	-55.6
benzeneacetamide	-1	DMSO	-54.0
benzenesulfonamide	-1	DMSO	-54.6
benzoic acid	-1	DMSO	-55.6
benzyl methyl ketone	-1	DMSO	-55.4
carbazole	-1	DMSO	-49.9
cyanamide	-1	DMSO	-59.5
cyanoacetophenone	-1	DMSO	-52.9
cyclopentadiene	-1	DMSO	-56.1
dichloroacetic acid	-1	DMSO	-49.2
dimethyl sulfone	-1	DMSO	-56.9
dimethyl sulfoxide	-1	DMSO	-55.4
diphenylamine	-1	DMSO	-47.7
ethanol	-1	DMSO	-64.6
formamide	-1	DMSO	-57.6
hydrobromic acid	-1	DMSO	-57.8
hydrochloric acid	-1	DMSO	-62.7
hydrogen cyanide	-1	DMSO	-54.0
imidazole	-1	DMSO	-56.7
isopropanol	-1	DMSO	-60.0
malononitrile	-1	DMSO	-46.0
methane sulfonamide	-1	DMSO	-57.5
methanol	-1	DMSO	-67.6
n-butanethiol	-1	DMSO	-55.7
nitromethane	-1	DMSO	-61.3
nitrous acid	-1	DMSO	-54.5
p-cresol	-1	DMSO	-53.9
phenol	-1	DMSO	-54.2
phenylacetylene	-1	DMSO	-56.4
phenylmalononitrile	-1	DMSO	-41.0
pyrazole	-1	DMSO	-54.2
succinimide	-1	DMSO	-58.6
t-butanol	-1	DMSO	-56.1

tetrazole	-1	DMSO	-54.5
thioacetamide	-1	DMSO	-54.9
thiophenol	-1	DMSO	-53.8
trifluoroacetamide	-1	DMSO	-49.2
trifluoroacetic acid	-1	DMSO	-45.0
urea	-1	DMSO	-58.9
water	-1	DMSO	-77.0
1-methylpiperidine	+1	methanol	-56.3
1-naphthaleneamine	+1	methanol	-69.6
2,6-dimethylpyridine	+1	methanol	-55.6
2-methylaniline	+1	methanol	-72.1
2-methylpyridine	+1	methanol	-57.7
3-bromoaniline	+1	methanol	-75.2
3-chloroaniline	+1	methanol	-76.0
3-methoxyaniline	+1	methanol	-68.0
3-methylaniline	+1	methanol	-71.3
3-methylpyridine	+1	methanol	-58.5
4-chloroaniline	+1	methanol	-75.5
4-cyanopyridine	+1	methanol	-72.1
4-ethylpyridine	+1	methanol	-57.6
4-methoxyaniline	+1	methanol	-72.1
4-methylaniline	+1	methanol	-71.7
4-methylpyridine	+1	methanol	-58.1
4-nitroaniline	+1	methanol	-75.3
4-phenylpyridine	+1	methanol	-62.3
ammonia	+1	methanol	-85.6
aniline	+1	methanol	-74.1
ethylamine	+1	methanol	-71.0
methylamine	+1	methanol	-74.3
n-butylamine	+1	methanol	-70.8
N-methylaniline	+1	methanol	-63.5
piperidine	+1	methanol	-62.9
pyridine	+1	methanol	-60.8
quinoline	+1	methanol	-57.5
triethylamine	+1	methanol	-53.0
trimethylamine	+1	methanol	-59.5
2,4-dinitrophenol	-1	methanol	-43.9
2-chlorobenzoic acid	-1	methanol	-64.1
2-chlorophenol	-1	methanol	-64.2
2-fluorobenzoic acid	-1	methanol	-67.5
2-fluorophenol	-1	methanol	-66.0
2-hydroxybenzoic acid	-1	methanol	-55.4
2-methoxyphenol	-1	methanol	-70.0
2-nitrobenzoic acid	-1	methanol	-62.2
2-t-butylphenol	-1	methanol	-61.6
3,4-dimethylbenzoic acid	-1	methanol	-72.1
3-chlorobenzoic acid	-1	methanol	-63.9
3-chlorophenol	-1	methanol	-64.0
3-cyanobenzoic acid	-1	methanol	-59.0
3-hydroxybenzoic acid	-1	methanol	-68.4
3-methoxybenzoic acid	-1	methanol	-67.7
3-methylbenzoic acid	-1	methanol	-68.2
3-nitrobenzoic acid	-1	methanol	-59.3
3-nitrophenol	-1	methanol	-58.9
3-trifluoromethylbenzoic acid	-1	methanol	-60.2
4-aminobenzoic acid	-1	methanol	-73.1
4-chlorobenzoic acid	-1	methanol	-63.9
4-fluorobenzoic acid	-1	methanol	-64.4
4-formylphenol	-1	methanol	-59.2
4-hydroxybenzoic acid	-1	methanol	-65.7
4-methoxybenzoic acid	-1	methanol	-69.0
4-methylbenzoic acid	-1	methanol	-68.6
4-nitrobenzoic acid	-1	methanol	-58.2
4-nitrophenol	-1	methanol	-54.1
4-t-butylbenzoic acid	-1	methanol	-67.4
4-t-butylphenol	-1	methanol	-68.0
acetic acid	-1	methanol	-72.9
acryclic acid	-1	methanol	-68.8
benzoic acid	-1	methanol	-67.5
bromoacetic acid	-1	methanol	-63.0

butanoic acid	-1	methanol	-71.4
chloroacetic acid	-1	methanol	-64.7
cyanoacetic acid	-1	methanol	-61.7
cyclobutanecarboxylic acid	-1	methanol	-71.3
cyclohexanecarboxylic acid	-1	methanol	-70.8
cyclopropanecarboxylic acid	-1	methanol	-71.7
dichloroacetic acid	-1	methanol	-59.3
fluoroacetic acid	-1	methanol	-67.2
glycolic acid	-1	methanol	-66.6
hydrobromic acid	-1	methanol	-65.8
hydrochloric acid	-1	methanol	-71.5
m-cresol	-1	methanol	-69.8
o-cresol	-1	methanol	-68.1
p-cresol	-1	methanol	-70.2
phenol	-1	methanol	-69.3
phenylacetic acid	-1	methanol	-69.5
propionic acid	-1	methanol	-72.0

Table S9. Values of Solvent Descriptors

solvent	n_{293K}	α	β	γ	ε	ϕ	ψ	N
acetic acid	1.3720	0.61	0.44	39.01	6.2528	0.000	0.000	7
acetonitrile	1.3442	0.07	0.32	41.25	35.6881	0.000	0.000	7
acetophenone	1.5372	0.00	0.48	56.19	17.4400	0.667	0.000	9
aniline	1.5863	0.26	0.41	60.62	6.8882	0.857	0.000	10
anisole	1.5174	0.00	0.29	50.52	4.2247	0.750	0.000	8
benzene	1.5011	0.00	0.14	40.62	2.2706	1.000	0.000	75
benzonitrile	1.5289	0.00	0.33	55.83	25.5920	0.750	0.000	7
benzyl alcohol	1.5396	0.33	0.56	52.96	12.4569	0.750	0.000	10
bromobenzene	1.5597	0.00	0.09	50.72	5.3954	0.857	0.143	27
bromoethane	1.4239	0.00	0.12	34.00	9.0100	0.000	0.333	7
bromoform	1.6005	0.15	0.06	64.58	4.2488	0.000	0.750	12
bromooctane	1.4524	0.00	0.12	41.28	5.0244	0.000	0.110	5
n-butanol	1.3993	0.37	0.48	35.88	17.3323	0.000	0.000	21
sec-butanol	1.3978	0.33	0.56	32.44	15.9436	0.000	0.000	9
butanone	1.3788	0.00	0.51	34.50	18.2457	0.000	0.000	13
butyl acetate	1.3941	0.00	0.45	35.81	4.9941	0.000	0.000	22
n-butylbenzene	1.4898	0.00	0.15	41.33	2.3600	0.600	0.000	10
sec-butylbenzene	1.4895	0.00	0.16	40.35	2.3446	0.600	0.000	5
t-butylbenzene	1.4927	0.00	0.16	39.78	2.3447	0.600	0.000	14
carbon disulfide	1.6319	0.00	0.07	45.45	2.6105	0.000	0.000	15
carbon tetrachloride	1.4601	0.00	0.00	38.04	2.2280	0.000	0.800	79
chlorobenzene	1.5241	0.00	0.07	47.48	5.6968	0.857	0.143	38
chloroform	1.4459	0.15	0.02	38.39	4.7113	0.000	0.750	109
chlorohexane	1.4199	0.00	0.10	37.03	5.9491	0.000	0.143	11
m-cresol	1.5438	0.57	0.34	51.37	12.4400	0.750	0.000	7
cyclohexane	1.4266	0.00	0.00	35.48	2.0165	0.000	0.000	92
cyclohexanone	1.4507	0.00	0.56	49.76	15.6186	0.000	0.000	10
decalin (mixture)	1.4528	0.00	0.00	43.82	2.1960	0.000	0.000	27
decane	1.4102	0.00	0.00	33.64	1.9846	0.000	0.000	39
decanol	1.4372	0.37	0.48	41.04	7.5305	0.000	0.000	11
1,2-dibromoethane	1.5387	0.10	0.17	56.93	4.9313	0.000	0.500	10
dibutyl ether	1.3992	0.00	0.45	35.98	3.0473	0.000	0.000	15
o-dichlorobenzene	1.5515	0.00	0.04	52.72	9.9949	0.750	0.250	11
1,2-dichloroethane	1.4448	0.10	0.11	45.86	10.1250	0.000	0.500	39
diethyl ether	1.3526	0.00	0.41	23.96	4.2400	0.000	0.000	72
diisopropyl ether	1.3679	0.00	0.41	24.86	3.3800	0.000	0.000	22
N,*N*-dimethylacetamide	1.4380	0.00	0.78	47.62	37.7807	0.000	0.000	7
N,*N*-dimethylformamide	1.4305	0.00	0.74	49.56	37.2190	0.000	0.000	7
2,6-dimethylpyridine	1.4953	0.00	0.63	44.64	7.1735	0.625	0.000	6
dimethyl sulfoxide	1.4170	0.00	0.88	61.78	46.8260	0.000	0.000	7
dodecane	1.4216	0.00	0.00	35.85	2.0060	0.000	0.000	8
ethanol	1.3611	0.37	0.48	31.62	24.8520	0.000	0.000	8
ethoxybenzene	1.5076	0.00	0.32	46.65	4.1797	0.667	0.000	7
ethyl acetate	1.3723	0.00	0.45	33.67	5.9867	0.000	0.000	24
ethylbenzene	1.4959	0.00	0.15	41.38	2.4339	0.750	0.000	29
fluorobenzene	1.4684	0.00	0.10	38.37	5.4200	0.857	0.143	7

1-fluoro-*n*-octane	1.3935	0.00	0.10	33.92	3.8900	0.000	0.111	6
heptane	1.3878	0.00	0.00	28.28	1.9113	0.000	0.000	69
heptanol	1.4249	0.37	0.48	38.50	11.3210	0.000	0.000	12
hexadecane	1.4345	0.00	0.00	38.93	2.0402	0.000	0.000	198
hexadecyl iodide	1.4806	0.00	0.15	46.48	3.5338	0.000	0.000	9
hexane	1.3749	0.00	0.00	25.75	1.8819	0.000	0.000	59
hexanol	1.4178	0.37	0.48	37.15	12.5102	0.000	0.000	14
iodobenzene	1.6200	0.00	0.12	55.72	4.5470	0.857	0.000	20
isobutanol	1.3955	0.37	0.48	32.38	16.7766	0.000	0.000	17
isooctane	1.3915	0.00	0.00	26.38	1.9358	0.000	0.000	32
isopropanol	1.3776	0.33	0.56	30.13	19.2645	0.000	0.000	7
isopropylbenzene	1.4915	0.00	0.16	39.85	2.3712	0.667	0.000	19
p-isopropyltoluene	1.4909	0.00	0.19	38.34	2.2322	0.600	0.000	6
mesitylene	1.4994	0.00	0.19	39.65	2.2650	0.667	0.000	7
methanol	1.3288	0.43	0.47	31.77	32.6130	0.000	0.000	0
methoxyethanol	1.4024	0.30	0.84	44.39	17.2000	0.000	0.000	6
methylene chloride	1.4242	0.10	0.05	39.15	8.9300	0.000	0.667	11
N-methylformamide	1.4319	0.40	0.55	55.44	181.5619	0.000	0.000	7
2-methylpyridine	1.4957	0.00	0.58	47.50	9.9533	0.714	0.000	6
4-methyl-2-pentanone	1.3962	0.00	0.51	33.83	12.8871	0.000	0.000	13
nitrobenzene	1.5562	0.00	0.28	57.54	34.8091	0.667	0.000	15
nitroethane	1.3917	0.02	0.33	46.25	28.2896	0.000	0.000	7
nitromethane	1.3817	0.06	0.31	52.58	36.5623	0.000	0.000	7
o-nitrotoluene	1.5450	0.00	0.27	59.12	25.6692	0.600	0.000	6
nonane	1.4054	0.00	0.00	32.21	1.9605	0.000	0.000	26
nonanol	1.4333	0.37	0.48	40.14	8.5991	0.000	0.000	10
octane	1.3974	0.00	0.00	30.43	1.9406	0.000	0.000	38
octanol	1.4295	0.37	0.48	39.01	9.8629	0.000	0.000	236
pentadecane	1.4315	0.00	0.00	38.34	2.0333	0.000	0.000	9
pentane	1.3575	0.00	0.00	22.30	1.8371	0.000	0.000	26
pentanol	1.4101	0.37	0.48	36.50	15.1300	0.000	0.000	22
perfluorobenzene	1.3777	0.00	0.00	31.74	2.0290	0.500	0.500	15
phenyl ether	1.5787	0.00	0.20	38.50	3.7300	0.923	0.000	6
propanol	1.3850	0.37	0.48	33.57	20.5237	0.000	0.000	7
pyridine	1.5095	0.00	0.52	52.62	12.9776	0.833	0.000	7
tetrachloroethene	1.5053	0.00	0.00	45.19	2.2680	0.000	0.667	10
tetrahydrofuran	1.4050	0.00	0.48	39.44	7.4257	0.000	0.000	7
tetrahydrothiophene dioxide	1.4833	0.00	0.88	87.49	43.9622	0.000	0.000	7
tetralin	1.5413	0.00	0.19	47.74	2.7710	0.600	0.000	9
toluene	1.4961	0.00	0.14	40.20	2.3741	0.857	0.000	51
tributylphosphate	1.4224	0.00	1.21	27.55	8.1781	0.000	0.000	16
triethylamine	1.4010	0.00	0.79	29.10	2.3832	0.000	0.000	7
1,2,4-trimethylbenzene	1.5048	0.00	0.19	42.03	2.3653	0.667	0.000	11
undecane	1.4398	0.00	0.00	34.85	1.9910	0.000	0.000	13
water	1.3328	0.82	0.35	103.62	78.3600	n.a.	n.a.	374
xylene (mixture)	1.4995	0.00	0.16	41.38	2.3879	0.750	0.000	48
1,2-dibromoethane/water	1.5387	0.10	0.17	56.93	4.9313	0.000	0.500	1
1,2-dichloroethane/water	1.4448	0.10	0.11	45.86	10.1250	0.000	0.500	3
benzene/water	1.5011	0.00	0.14	40.62	2.2706	1.000	0.000	4
carbon tetrachloride/water	1.4601	0.00	0.00	38.04	2.2280	0.000	0.800	2

chlorobenzene/water	1.5241	0.00	0.07	47.48	5.6968	0.857	0.143	1
chloroform/water	1.4459	0.15	0.02	38.39	4.7113	0.000	0.750	7
cyclohexane/water	1.4266	0.00	0.00	35.48	2.0165	0.000	0.000	5
dibutyl ether/water	1.3992	0.00	0.45	35.98	3.0473	0.000	0.000	1
diethyl ether/water	1.3526	0.00	0.41	23.96	4.2400	0.000	0.000	8
ethyl acetate/water	1.3723	0.00	0.45	33.67	5.9867	0.000	0.000	1
heptane/water	1.3878	0.00	0.00	28.28	1.9113	0.000	0.000	6
hexane/water	1.3749	0.00	0.00	25.75	1.8819	0.000	0.000	1
nitrobenzene/water	1.5562	0.00	0.28	57.54	34.8091	0.667	0.000	1
octanol/water	1.4295	0.37	0.48	39.01	9.8629	0.000	0.000	103

[a] Solvent descriptors: refractive index (n_{293K}); Abraham's hydrogen bond acidity parameter (α); Abraham's hydrogen bond basicity parameter (β); macroscopic surface tension in cal mol^{-1} Å^{-2} (γ); dielectric constant at 298.15K (ε); fraction of non-hydrogenic solvent atoms that are aromatic carbon atoms (carbon aromaticity, ϕ); fraction of non-hydrogenic atoms in the solvent molecule that are F, Cl, or Br (electronegative halogenicity, ψ). *N* is the number of neutral solute data in a given solvent.

Table S10. Mean Signed Errors (in kcal/mol) [a]

		SM12CM5				SM12ESP/MG3S					
		B3LYP		M06-2X		MK		ChElPG			
solute class	*N*	MG3S	6-31G(d)	MG3S	6-31G(d)	B3LYP	M06-2X	B3LYP	M06-2X	SM8	SMD
					274 aqueous data						
H_2, NH_3, H_2O, $(H_2O)_2$	4	–1.26	–1.78	–1.33	–1.82	–1.29	–1.36	–1.16	–1.24	–1.92	–1.60
hydrocarbons	40	–0.59	–0.72	–0.65	–0.75	–1.00	–1.23	–0.33	–0.49	–0.50	–0.20
alcohols and phenols	16	0.73	0.31	0.62	0.23	0.00	–0.18	0.45	0.32	0.59	–0.02
ethers	12	–0.02	–0.33	–0.16	–0.43	0.02	–0.23	0.40	0.19	0.35	0.41
aldehydes and ketones	18	–0.13	–0.37	–0.20	–0.40	–0.52	–0.45	–0.34	–0.24	–0.17	–0.04
carboxylic acids	5	0.98	0.56	0.87	0.49	0.21	0.19	0.24	0.23	0.72	0.62
esters	13	–0.05	–0.44	–0.18	–0.52	–0.68	–0.75	–0.46	–0.51	–0.22	–0.15
peroxides	3	0.38	–0.24	0.20	–0.38	–0.05	–0.26	0.03	–0.18	0.10	–1.12
bifunctional HCO compounds	5	0.54	0.05	0.44	0.00	–0.86	–1.15	0.07	–0.13	0.79	0.19
aliphatic amines	15	0.44	0.25	0.37	0.21	–0.31	–0.41	–0.02	–0.08	0.12	0.41
anilines	7	0.75	0.19	0.64	0.15	0.21	–0.38	1.86	1.40	0.47	–0.09
aromatic nitrogen heterocycles, including 1-methylthymine	13	0.44	–0.03	0.34	–0.11	–0.43	–0.63	0.58	0.45	–0.14	0.38
nitriles	4	0.21	–0.17	0.23	–0.08	–0.74	–0.50	–0.49	–0.21	0.31	0.65
hydrazines	3	–0.02	–0.42	–0.12	–0.48	0.18	–0.01	0.80	0.60	–0.29	–0.22
bifunctional HCN compounds	3	1.75	0.95	1.60	0.86	–0.26	–0.48	1.36	1.16	0.38	–0.14
amides, ureas	6	0.09	–0.69	–0.09	–0.82	–0.23	–0.42	0.28	0.14	–0.16	0.90
nitrohydrocarbons	7	–0.68	–1.07	–0.96	–1.35	–1.38	–1.52	–1.17	–1.29	–0.45	0.12
bifunctional HCNO compounds	3	0.05	–0.30	–0.09	–0.40	–0.63	–0.86	–0.40	–0.61	0.03	–0.02
compounds containing H, C, and F	6	–0.38	–0.49	–0.47	–0.58	–0.26	–0.36	–0.19	–0.26	–0.40	0.17
compounds containing H, C, and Cl	27	–0.09	–0.31	–0.17	–0.38	–0.81	–1.00	–0.40	–0.53	0.05	–0.30
compounds containing H, C, and Br	14	–0.10	–0.24	–0.13	–0.29	–0.41	–0.51	0.04	–0.05	–0.29	–0.53
multihalogen (F, Cl, or Br) hydrocarbons	12	–0.30	–0.40	–0.36	–0.46	–0.33	–0.38	–0.29	–0.34	–0.13	0.19
halogen (F, Cl, or Br) compounds containing H, C, N, and/or O	9	0.95	0.55	0.84	0.46	0.51	0.42	0.67	0.63	1.12	0.71
sulfur compounds not containing P	14	0.29	0.05	0.22	–0.01	–0.34	–0.50	0.16	0.05	0.48	0.03
phosphorus compounds	14	0.30	–0.51	0.07	–0.72	–0.34	–0.61	0.20	–0.03	–0.12	0.09
silicon compound	1	–0.26	–0.28	–0.27	–0.28	–0.98	–0.97	–0.74	–0.68	–0.16	0.65
all data	274	0.05	–0.27	–0.04	–0.34	–0.48	–0.63	–0.01	–0.13	–0.01	0.01
					66 aqueous data (SAMPL1)						
compounds containing H, C, and O	9	0.04	–0.45	–0.14	–0.57	–0.25	–0.41	–0.11	–0.23	0.15	–0.27
compounds containing H, C, N, and/or O	18	–0.17	–0.84	–0.30	–0.90	–0.43	–0.56	0.27	0.21	0.27	0.82
halogen (F, Cl, or Br) compounds containing H, C, N, and/or O	19	1.34	0.85	1.21	0.74	0.91	1.03	0.94	1.05	1.54	1.17
sulfur compounds not containing P	9	0.30	–0.41	0.11	–0.56	0.07	0.03	0.36	0.30	–1.60	–0.76
phosphorus compounds	11	0.76	–0.13	0.54	–0.30	–0.04	–0.26	0.76	0.55	–0.55	–0.71
all data	66	0.51	–0.12	0.35	–0.24	0.11	0.05	0.51	0.46	0.23	0.30

Table S10. Continued

		SM12CM5				SM12ESP/MG3S					
		B3LYP		M06-2X		MK		ChElPG			
solute class	*N*	MG3S	6-31G(d)	MG3S	6-31G(d)	B3LYP	M06-2X	B3LYP	M06-2X	SM8	SMD
		26 aqueous data (SAMPL2)									
all data	26	0.88	0.21	0.72	0.09	0.00	−0.10	0.34	0.31	0.89	1.61
		8 aqueous data (iodine compounds)									
all data	8	−0.35	−0.34	−0.45	−0.41	−0.59	−0.62	−0.08	−0.15		
		2129 nonaqueous data (including iodine compounds)									
H_2, NH_3, H_2O	29	−1.22	−1.40	−1.25	−1.42	−1.01	−1.05	−0.96	−1.01	−1.49	−1.08
hydrocarbons	266	−0.11	−0.23	−0.17	−0.27	−0.34	−0.61	0.30	0.11	−0.15	−0.19
alcohols and phenols	381	0.19	0.04	0.14	0.00	−0.08	−0.20	0.24	0.15	0.14	0.04
ethers	87	0.24	0.09	0.16	0.03	0.09	−0.03	0.30	0.20	0.14	0.15
aldehydes and ketones	227	−0.25	−0.30	−0.28	−0.32	−0.31	−0.30	−0.21	−0.19	−0.64	−0.53
carboxylic acids	120	0.23	0.10	0.18	0.06	0.06	0.05	0.08	0.06	0.41	0.37
esters, including lactones	243	0.02	−0.07	−0.02	−0.10	−0.08	−0.11	−0.01	−0.04	0.13	0.15
peroxides	17	0.15	−0.09	0.08	−0.14	0.27	0.20	0.26	0.18	−0.08	−0.05
bifunctional HCO compounds	32	1.24	0.89	1.16	0.85	0.60	0.34	1.29	1.12	1.22	1.08
aliphatic amines	154	0.26	0.14	0.23	0.12	−0.18	−0.16	0.01	0.03	0.17	0.08
anilines	61	0.14	−0.25	0.07	−0.28	−0.12	−0.55	1.06	0.72	0.07	−0.17
aromatic nitrogen heterocycles, including 1-methylthymine and uracil	66	0.16	−0.14	0.08	−0.20	−0.47	−0.68	0.37	0.21	−0.08	0.31
nitriles	20	−0.04	−0.24	−0.03	−0.18	−0.82	−0.76	−0.41	−0.30	−0.20	−0.50
hydrazines	5	−0.04	−0.39	−0.11	−0.42	0.36	0.28	0.82	0.70	0.05	−0.14
bifunctional HCN compounds	2	0.04	−0.95	−0.21	−1.15	−1.96	−2.17	−0.46	−0.70	−1.39	−1.55
amides, ureas, and lactams	37	−0.33	−0.65	−0.43	−0.72	−0.21	−0.38	0.14	0.01	0.21	0.60
nitrohydrocarbons	86	0.14	−0.09	−0.08	−0.31	−0.12	−0.35	0.03	−0.18	−0.46	−0.13
bifunctional HCNO compounds	7	0.15	−0.31	0.06	−0.36	−0.02	−0.02	0.29	0.33	0.48	1.81
compounds containing H, C, and F	17	−0.02	−0.08	−0.07	−0.13	−0.42	−0.60	−0.05	−0.18	−0.04	−0.38
compounds containing H, C, and Cl	74	−0.16	−0.28	−0.22	−0.32	−0.47	−0.58	−0.27	−0.35	0.01	−0.22
compounds containing H, C, and Br	39	−0.44	−0.53	−0.47	−0.56	−0.62	−0.72	−0.27	−0.36	−0.58	−0.64
multihalogen (F, Cl, or Br) hydrocarbons	14	−0.76	−0.78	−0.78	−0.80	−0.68	−0.71	−0.66	−0.69	−0.31	0.23
halogen (F, Cl, or Br) compounds containing H, C, N, and/or O	52	1.11	0.85	1.03	0.77	0.59	0.43	0.95	0.84	1.45	1.29
sulfur compounds not containing P	33	0.18	0.04	0.12	−0.02	−0.22	−0.37	0.22	0.09	−0.16	−0.26
phosphorus compounds	37	0.12	−0.25	−0.02	−0.39	−0.39	−0.55	−0.10	−0.27	0.24	0.31
silicon compounds	2	1.73	1.72	1.72	1.71	1.11	1.15	1.27	1.33	1.63	1.81
iodine compounds	21	0.03	−0.02	−0.06	−0.08	−0.21	−0.31	0.24	0.14		
all data	2129	0.07	−0.09	0.01	−0.13	−0.18	−0.29	0.14	0.05	0.00	0.00

Table S10. Continued

		SM12CM5				SM12ESP/MG3S					
		B3LYP		M06-2X		MK		ChElPG			
solute class	*N*	MG3S	6-31G(d)	MG3S	6-31G(d)	B3LYP	M06-2X	B3LYP	M06-2X	SM8	SMD
					144 transfer energy data						
hydrocarbons	2	–0.29	–0.24	–0.27	–0.23	–0.18	–0.12	–0.34	–0.30	0.07	0.79
lactones	10	–0.59	–0.27	–0.52	–0.21	0.28	0.19	0.44	0.33	0.02	0.06
aromatic nitrogen heterocycles	7	–0.47	–0.34	–0.45	–0.32	0.00	0.07	–0.35	–0.31	–0.02	0.15
bifunctional HCN compounds	4	0.24	0.33	0.24	0.32	0.64	0.61	0.57	0.54	0.41	0.57
amides, ureas, and lactams	28	–1.03	–0.72	–0.97	–0.67	–0.76	–0.74	–0.90	–0.90	–0.49	–0.65
thymines or uracils	7	–0.12	0.20	–0.08	0.23	0.49	0.34	0.44	0.28	0.44	–0.31
bifunctional HCNO compounds	5	0.20	0.33	0.21	0.34	0.57	0.53	0.53	0.49	0.14	0.46
halogen (F, Cl, or Br) compounds containing H, C, N, and/or O	38	0.20	0.36	0.23	0.39	0.42	0.42	0.41	0.41	0.55	0.30
sulfur compounds not containing P	21	–0.05	0.07	–0.04	0.08	0.09	0.09	0.06	0.05	0.01	0.00
phosphorus compounds	9	–0.41	0.04	–0.26	0.18	0.62	0.77	0.54	0.64	–0.56	0.50
silicon compounds	13	0.18	0.23	0.20	0.24	0.21	0.25	0.12	0.15	0.28	0.08
all data	144	–0.23	–0.02	–0.18	0.02	0.11	0.12	0.05	0.04	0.08	0.03
					112 selectively clustered ions in water						
anions	60	1.57	0.46	1.19	0.12	0.17	–0.24	1.21	0.84	0.14	4.09
cations	52	3.07	2.25	2.99	2.15	2.61	2.58	2.84	2.85	0.47	2.68
all data	112	2.27	1.29	2.03	1.06	1.30	1.07	1.97	1.77	0.29	3.44
					80 ions in methanol						
anions	51	–0.61	–1.84	–1.12	–2.39	–1.94	–2.33	–1.19	–1.49	–2.28	0.46
cations	29	0.80	–0.25	0.64	–0.46	0.34	0.11	0.77	0.62	–1.32	–0.45
all data	80	–0.10	–1.27	–0.48	–1.69	–1.12	–1.44	–0.48	–0.72	–1.93	0.13
					69 ions in acetonitrile						
anions	30	–3.97	–4.42	–4.21	–4.68	–3.19	–3.56	–2.62	–2.91	–4.50	–3.58
cations	39	6.92	6.18	6.87	6.09	6.47	6.48	6.58	6.61	5.06	7.69
all data	69	2.19	1.57	2.05	1.41	2.27	2.12	2.58	2.47	0.90	2.79
					71 ions in dimethyl sulfoxide						
anions	67	–5.88	–6.52	–6.11	–6.74	–6.17	–6.55	–4.95	–5.27	–7.52	–3.52
cations	4	–1.50	–2.20	–1.59	–2.29	–1.23	–1.53	–0.69	–0.92	–1.52	8.35
all data	71	–5.63	–6.27	–5.86	–6.49	–5.89	–6.26	–4.71	–5.02	–7.18	–2.86

[a] The table shows mean signed errors (relative to reference data) in solvation free energies and transfer free energies computed at the SM12/DFT/MG3S and SM12/DFT/6-31G(d) level of theory using CM5 charges and at the SM12/DFT/MG3S level using Merz–Kollman (MK) and ChElPG charges where DFT is B3LYP and M06-2X. The errors in the SM8/CM4M/M06-2X/6-31G(d) and SMD/M05-2X/6-31G(d) solvation energies are also reported. Iodine-containing compounds are not included in the SM8 and SMD statistics. See the main text for further details.

Section S11

Functional Forms for the G_{CDS} Contribution

The cavity–dispersion–solvent-structure (CDS) contribution, G_{CDS}, to the free energy of solvation is defined as

$$G_{CDS} = \sum_{k}^{atoms} \sigma_k A_k(\mathbf{R}, \{R_{Z_k} + r_s\}) + \sigma^{[M]} \sum_{k}^{atoms} A_k(\mathbf{R}, \{R_{Z_k} + r_s\})$$

where σ_k is the atomic surface tension of atom k, A_k is the solvent-accessible surface area (SASA) of atom k, and $\sigma^{[M]}$ is the molecular surface tension. The SASA depends on the geometry **R**, the set $\{R_{Z_k}\}$ of atom-number-dependent van der Waals radii, and the solvent radius r_s added to each of R_{Z_k}. The quantities σ_k are defined by the following equation

$$\sigma_k = \tilde{\sigma}_{Z_k} + \sum_{k'}^{atoms} \tilde{\sigma}_{Z_k Z_{k'}} T_k(\{Z_{k'}, R_{kk'}\})$$

where $\tilde{\sigma}_Z$ is a quantity that depends on the atomic number of atom k, $\tilde{\sigma}_{ZZ'}$ is a quantity that depends on the atomic numbers of atoms k and k', and $T_k(\{Z_{k'}, R_{kk'}\})$ is a geometry-dependent switching function called a cutoff tanh, or COT. We describe the quantities σ_k in more detail below. For convenience of tabulation, atomic numbers are replaced with atomic symbols.

For Z_k = H

$$\sigma_k = \tilde{\sigma}_{H} + \tilde{\sigma}_{HC} \sum_{\substack{k' \\ Z_{k'}=C}}^{atoms} T(R_{kk'}, r_{HC}, \Delta r_{HC}) + \tilde{\sigma}_{HN} \sum_{\substack{k' \\ Z_{k'}=N}}^{atoms} T(R_{kk'}, r_{HN}, \Delta r_{HN}) + \tilde{\sigma}_{HO} \sum_{\substack{k' \\ Z_{k'}=O}}^{atoms} T(R_{kk'}, r_{HO}, \Delta r_{HO})$$

For $Z_k = \mathrm{C}$

$$\sigma_k = \widetilde{\sigma}_{\mathrm{C}} + \widetilde{\sigma}_{\mathrm{CC}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{C} \\ k' \neq k}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{CC}}, \Delta r_{\mathrm{CC}}) + \widetilde{\sigma}_{\mathrm{CN}} \left[\sum_{\substack{k' \\ Z_{k'}=\mathrm{N}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{CN}}, \Delta r_{\mathrm{CN}}) \right]^2 +$$

$$\widetilde{\sigma}_{\mathrm{CO2}} \left\{ \sum_{\substack{k' \\ Z_{k'}=\mathrm{O}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{CO}}, \Delta r_{\mathrm{CO}}) \left[\sum_{\substack{k'' \\ Z_{k''}=\mathrm{O} \\ k'' \neq k'}}^{\text{atoms}} T(R_{k\,k''}, r_{\mathrm{CO}}, \Delta r_{\mathrm{CO}}) \right] \right\}$$

For $Z_k = \mathrm{N}$

$$\sigma_k = \widetilde{\sigma}_{\mathrm{N}} + \widetilde{\sigma}_{\mathrm{NC}} \left\{ \sum_{\substack{k' \\ Z_{k'}=\mathrm{C}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{NC}}, \Delta r_{\mathrm{NC}}) \left[\sum_{\substack{k'' \\ k'' \neq k' \\ k'' \neq k}}^{\text{atoms}} T(R_{k'k''}, r_{\mathrm{C}Z_{k''}}, \Delta r_{\mathrm{C}Z_{k''}}) \right]^2 \right\}^{1.3} +$$

$$\widetilde{\sigma}_{\mathrm{NC2}} \left\{ \sum_{\substack{k' \\ Z_{k'}=\mathrm{C}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{NC}}, \Delta r_{\mathrm{NC}}) \left[\sum_{\substack{k'' \\ Z_{k''}=\mathrm{O}}}^{\text{atoms}} T(R_{k'k''}, r_{\mathrm{CO}}, \Delta r_{\mathrm{CO}}) \right] \right\}$$

For $Z_k = \mathrm{O}$

$$\sigma_k = \widetilde{\sigma}_{\mathrm{O}} + \widetilde{\sigma}_{\mathrm{OC}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{C}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{OC}}, \Delta r_{\mathrm{OC}}) + \widetilde{\sigma}_{\mathrm{ON}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{N}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{ON}}, \Delta r_{\mathrm{ON}}) +$$

$$\widetilde{\sigma}_{\mathrm{OO}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{O} \\ k' \neq k}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{OO}}, \Delta r_{\mathrm{OO}}) + \widetilde{\sigma}_{\mathrm{OP}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{P}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{OP}}, \Delta r_{\mathrm{OP}}) + \widetilde{\sigma}_{\mathrm{OS}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{S}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{OS}}, \Delta r_{\mathrm{OS}})$$

For $Z_k = \mathrm{S}$

$$\sigma_k = \widetilde{\sigma}_{\mathrm{S}} + \widetilde{\sigma}_{\mathrm{SP}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{P}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{SP}}, \Delta r_{\mathrm{SP}})$$

For $Z_k \neq$ H, C, N, O, S

$$\sigma_k = \widetilde{\sigma}_{Z_k}$$

The function $T(R_{kk'}, r_{Z_k Z_{k'}}, \Delta r_{Z_k Z_{k'}})$ is a geometry-dependent switching function called a cutoff tanh. This function is described as follows

$$T(R_{kk'}, r_{Z_k Z_{k'}}, \Delta r_{Z_k Z_{k'}}) = \begin{cases} \exp\left(\dfrac{\Delta r_{Z_k Z_{k'}}}{R_{kk'} - \Delta r_{Z_k Z_{k'}} - r_{Z_k Z_{k'}}} \right) & \text{if } R_{kk'} < r_{Z_k Z_{k'}} + \Delta r_{Z_k Z_{k'}} \\ 0 & \text{otherwise} \end{cases}$$

where $R_{kk'}$ is the interatomic distance between atoms *k* and *k*′ and $r_{Z_k Z_{k'}}$ and $\Delta r_{Z_k Z_{k'}}$ are atomic-number-specific parameters described in Table S11.

Table S11. Values of $r_{ZZ'}$ and $\Delta r_{ZZ'}$ (Å) [a]

ZZ'	$r_{ZZ'}$	$\Delta r_{ZZ'}$
HC	1.55	0.3
HN	1.55	0.3
HO	1.55	0.3
CH	1.55	0.3
CC	1.84	0.3
CN	1.84	0.3
CO	1.84	0.3
CF	1.84	0.3
CP	2.2	0.3
CS	2.2	0.3
CCl	2.1	0.3
CBr	2.3	0.3
CI	2.6	0.3
C*X*	2.1	0.3
NC	1.84	0.3
OC	1.33	0.1
ON	1.5	0.3
OO	1.8	0.3
OP	2.1	0.3
OS	1.71	0.3
SP	2.5	0.3

[a] Any possible $r_{ZZ'}$ or $\Delta r_{ZZ'}$ that is not in the table is set equal to zero. *X* refers to any element other than H, C, N, O, F, P, S, Cl, Br, and I.