Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Footprinting Molecular Electrostatic Potential Surfaces for Calculation of Solvation Energies

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Supplementary Information

Table S1. H-bond acceptor parameters.

Compound Name	***β***
Propionyl fluoride	2.8
Benzoyl fluoride	2.4
Diethylcarbamoyl chloride	5.5
Dimethylcarbomyl chloride	5.3
Diphenylcarbamoyl chloride	4.7
Methanol	4.8
Ethanol	5.2
Propan-2-ol	5.5
tert-Butyl alcohol	5.7
2-Chloroethanol	4.2
2,2,2-Trifluoroethanol	2.5
Hexafluoropropan-2-ol	0.9
Water	4.5
2,2,2-Trichloroethanol	2.8
2-Fluoroethanol	4.3
Benzyl alcohol	4.9
Octan-1-ol	5.4
Cyclohexanol	5.6
Adamantan-1-ol	5.9
Phenylethanol	5.3
Ethylene glycol	5.3
Allylalcohol	4.8
Prop-2-yn-1-ol	3.7
2-Bromoethanol	4.2
Propan-1-ol	5.3
N-Acetylpiperidine	8.2
N-Chloroacetylpiperidine	7.0
N,N-Diphenylpropanamide	6.9
N,N-Diphenylbutanamide	7.1
N,N-Diphenylchloroacetamide	6.2
N,N-Diethylbenzamide	7.8
N,N-Dicyclohexylbenzamide	8.0
N-Benzoylpiperidine	7.9
N,N-Diethyl-4-nitrobenzamide	7.0
N,N-Dicyclohexyl-4-nitrobenzamide	6.9
N,N-Diethylpropanamide	7.7
4-Nitro-N,N-diphenylbenzamide	5.9

N-Phenylpyrrolidin-2-one	7.1
3-Methyl-4-pyrimidone	7.2
N-Propionylpiperidine	8.0
N,N-Diethylbutanamide	7.9
N-Butyrylpiperidine	8.0
1-Chloro-N,N-diethylacetamide	7.0
1,1-Dichloro-N,N-diethylacetamide	6.2
1-Chloro-N,N-dicyclohexylacetamide	6.9
N-(3-Methoxyphenyl)pyrrolidin-2-one	7.0
N-(4-Methylphenyl)pyrrolidin-2-one	7.3
N-(4-Ethylphenyl)pyrrolidin-2-one	7.3
N-(4-Chlorophenyl)pyrrolidin-2-one	6.5
N-(4-Methoxyphenyl)pyrrolidin-2-one	7.5
1,3-Dimethyluracil	7.0
N-(2-Chlorophenyl)pyrrolidin-2-one	7.8
N-(2-Methoxyphenyl)pyrrolidin-2-one	8.1
N-(3-Methylphenyl)pyrrolidin-2-one	7.2
N-(3-Chlorophenyl)pyrrolidin-2-one	6.4
Pyrrolidin-2-one	8.9
N,N-Diethylnonamide	7.9
N,N-Dimethylsobutylamide	7.9
1,1,1-Trichloro-N,N-Diethylacetamide	5.7
1,1,1-Trifluoro-N,N-Diethylacetamide	5.5
N,N-Dimethyl-4-bromobenzamide	7.7
1-Formylpiperidine	7.7
N,N-Diethylformamide	7.7
N,N-Dimethyl-4-fluorobenzamide	7.8
N,N-Dimethyl-2,2,2-trichloroacetamide	5.7
N,N-Diphenylformamide	6.2
N,N-Diphenylbenzamide	6.6
N,N-Diphenyl-2,2-dimethylpropionamide	6.7
N,N-Diphenyl-4-methoxybenzamide	6.8
N,N-Dimethyl-4-nitrobenzamide	7.3
N,N-Dimethyl-4-(triflouromethyl)benzamide	7.4
N,N-Dimethyl-4-methylbenzamide	8.1
1,1,3,3-Tetraphenylurea	6.9
1,1-Diphenyl-3,3-diethylurea	7.7
1,1-Diphenyl-3,3-dimethylurea	7.7
1,3-Diphenyl-1,3-diethylurea	7.9
N,N-Dimethyl-4-methoxybenzamide	8.2
N,N-Diethyl-4-methoxybenzamide	8.3
N,N-Dimethyl-4-dimethylaminobenzamide	8.6
Phenyl diphenylcarbamate	5.7
Methyl diphenylcarbamate	6.2
Ethyl diphenylcarbamate	6.3
Methyl dimethylcarbamate	7.1
Ethyl diethylcarbamate	7.4
N-Methylformamide	7.4
N,N-Diphenylacetamide	7.4
N,N-Diisopropyl-2,2-dimethylpropionamide	7.6
N,N-Dicyclohexyl-2,2-dimethylpropionamide	7.6
N,N-Dimethylformamide	7.7

N-Methylacetanilide	7.9
N,N-Dicyclohexylpropionamide	8.0
N-Ethylacetamide	8.1
N,N-Dimethyl-2,2,2-trifluoroacetamide	5.4
N,N-Dimethylbenzamide	8.0
1-Methyl-2-pyridone	8.8
1-Methyl-2-piperidone	8.8
N,N-Dimethyl methylamide phenyl ether	6.8
Ethyl dimethylcarbamate	7.1
1,1,3,3-Tetraethylurea	8.5
1,1,3,3-Tetramethylurea	8.5
N,N'-Dimethyl N,N'-ethyleneurea	8.5
N,N'-Dimethyl N,N'-trimethyleneurea	9.3
N,N-Dicyclohexylisobutyramide	8.0
N,N-Dicyclohexylacetamide	8.4
N,N-Dimethylacetamide	8.5
1-methyl-2-pyrrolidone	8.3
N-Methylcaprolactam	8.7
N,N-Dimethylisopropylamide	8.1
N,N-Dimethylpropionamide	8.3
N,N-Diethylacetamide	8.5
N,N-Dimethyltertbutylamide	7.7
N-Methylpropionamide	8.0
N,N-Dimethyl-2-chloroacetamide	6.9
N-Methylformanilide	6.9
N-Methylbenzamide	7.6
N-Methylacetamide	8.2
N-Methylsuccinimide	6.1
N',N'-Diphenyl acetamidine	6.7
N,N tert-butyl methyl tert butylamide	7.6
ε-Caprolactam	6.7
Z-benzyl, 2-benzisothiazol-3(2H)-one 1,1 dioxide	4.6
N-Methyl-3-isooxazolidinone	7.0
N-Methylmaleimide	5.8
Pentylacetylene	2.7
Butylacetylene	2.4
Hexylacetylene	2.9
Hexa-1,2-diene	1.7
Styrene	2.5
Ethyl benzene	2.2
Decyl benzene	2.4
Benzene	2.1
Phenanthrene	2.9
Toluene	2.1
o-Xylene	2.3
m-Xylene	2.4
p-Xylene	2.5
Mesitylene	2.7
1,2,4,5-Tetramethylbenzene	2.7
Hexamethylbenzene	3.3
Naphthalene	2.8
Pentamethylbenzene	2.8

Biphenyl	2.7
Cyclohexene	1.2
1-Methylpyrrole	3.6
Pyrrole	4.1
Triphenylarsine	3.6
4-Nitrobenzaldehyde	3.9
1,3-Dichloropropan-2-one	4.2
Propanaldehyde	4.6
Butanaldehyde	4.7
Octanaldehyde	4.6
Decanaldehyde	4.7
2-Methoxybenzaldehyde	5.5
Acetaldehyde	4.5
Benzaldehyde	4.8
4-Chlorobenzaldehyde	4.5
4-Methoxybenzaldehyde	5.5
4-(Dimethylamino)benzaldehyde	6.5
trans-Cinnamaldehyde	5.6
Mesityl oxide	5.8
Piperitone	6.1
Hexafluoropropanone	2.6
Pentan-3-one	5.6
3-Methylpentan-2-one	5.8
4-Methylpentan-2-one	5.7
2,4-Dimethylpentan-3-one	5.5
Hexan-3-one	5.6
Heptan-4-one	5.6
2,6-Dimethylheptan-4-one	5.4
3,5-Dimethylheptan-4-one	5.4
Butan-2-one	5.8
Biacetyl	4.2
Acetyl acetone	5.1
1,1-Dichloropropan-2-one	3.6
Chloropropan-2-one	4.5
Dicyclopropyl ketone	6.1
3-Methylbutan-2-one	5.7
Pentan-2-one	5.7
2,2,4,4-Tetramethylpentan-3-one	5.2
Hexan-2-one	5.7
1-Adamantyl methyl ketone	6.0
Cyclohexyl methyl ketone	5.8
Methyl cyclopropyl ketone	6.0
Propan-2-one	5.7
Cycloundecanone	5.7
Cyclododecanone	5.8
Cyclopentadecanone	5.8
Camphor	6.0
Benzil	4.7
1,4-Benzoquinone	4.9
9,10-Phenanthrequinone	5.3
1,1,1-Trifluoropropan-2-one	2.9
1-Adamantyl tert-butyl ketone	5.5

1,1,1-Trichloropropan-2-one	3.1
γ-Pyrone	7.6
2,6-Dimethyl-γ-pyrone	8.6
Di-(1-adamantyl)ketone	5.7
Cyclobutanone	5.3
Cyclopentanone	5.9
Cyclohexanone	6.2
2-Methylcyclohexanone	5.9
Cycloheptanone	6.2
Cyclooctanone	6.3
Xanthone	6.1
4-Aminoacetophenone	6.4
4-Methoxyacetophenone	6.0
4-(1-Adamantyl)acetophenone	6.0
4-tert-Butylacetophenone	5.8
4-Isopropylacetophenone	5.8
4-Ethylacetophenone	5.8
4-Methylacetophenone	5.8
4-Methylthioacetophenone	5.8
Acetophenone	5.5
4-Fluoroacetophenone	5.3
Flavone	7.5
4-Chloroacetophenone	5.1
1,4-Diacetylbenzene	5.8
4-Cyanoacetophenone	5.2
4-(Trifluoromethyl)acetophenone	4.8
4-Nitroacetophenone	4.6
3-Methoxyacetophenone	5.6
3-Methylacetophenone	5.5
3-(Trifluoromethyl)acetophenone	4.7
Anthrone	5.6
Thioxanthen-9-one	5.7
10-Methyl-9(10H)-acridone	7.3
4-(Diethylamino)acetophenone	7.1
4-(Dimethylamino)acetophenone	7.0
4-Piperidinoacetophenone	6.9
4-Morpholinoacetophenone	6.6
3-Fluoroacetophenone	4.9
4-(Dimethylamino)benzophenone	7.0
4,4'-Bis(dimethylamino)benzophenone	7.3
4,4'-Bis(diethylamino)benzophenone	8.2
Dimesityl ketone	5.3
But-3-yn-2-one	4.6
9-Fluorenone	5.5
2-Acetylnaphthalene	5.6
3-Chloro-5,5-dimethylcyclohexenone	5.8
trans-4-Phenylbut-3-en-2-one	6.1
3-Methyl-5,5-dimethylcyclohexenone	6.9
3-Chloroacetophenone	4.9
Tropone	7.4
Diphenylcyclopropenone	8.2
N-Methylquinol-4-one	9.8

3-Dimethylamino-5,5-dimethylcyclohexenone	9.5
Dibenzyl ketone	5.3
Benzotropone	7.2
α,α'-Dimethylbenzotropone	6.4
α,α'-Diphenylbenzotropone	6.0
1,3-Diacetylbenzene	5.6
3-Nitroacetophenone	4.6
2-Chloroacetophenone	5.1
2-Methoxyacetophenone	6.0
Benzophenone	5.4
4-Methoxybenzophenone	5.9
4,4'-Bis(methoxy)benzophenone	6.4
Methyl isopropyl ketone	5.6
Benzoic acid	4.9
Butanoic acid	4.9
Acetic anhydride	6.4
Methyl formate	4.5
Vinyl acetate	4.7
Methyl ethanoate	4.7
Methyl salicylate	3.8
Ethyl 3-dimethylaminoacrylate	7.7
Methyl-cyclopropanecarboxylate	5.6
Ethyl isovalerate	5.5
Methyl cyclohexanecarboxylate	5.4
4-Nitrophenyl acetate	3.8
Propyl ethanoate	5.6
Butyl acetate	5.6
Isobutyl acetate	5.6
sec-Butyl acetate	5.6
Ethyl butyrate	5.5
S-Ethyl methylcarbonate	4.7
tert-Butyl benzoate	5.2
Ethyl 4-fluorobenzoate	5.0
Ethyl 3-methylbenzoate	5.3
Phenylformate	4.5
Ethyl chloroacetate	4.6
Ethyl flouroacetate	4.7
Ethyl isobutyrate	5.5
Ethyl cyclopropanecarboxylate	5.6
(E)-Ethyl cinnamate	5.6
β-Propiolactone	5.0
β-Butyrolactone	5.2
γ-Butyrolactone	6.0
γ-Valerolactone	6.2
Coumarin	6.0
δ-Valerolactone	6.6
Diethyl oxalate	4.5
Triacetin	4.9
Ethyl 4-bromobenzoate	4.8
Ethyl propiolate	4.5
Ethyl formate	4.5
Methyl benzoate	5.0

Ethyl benzoate	5.2
Ethyl 4-methylbenzoate	5.4
Ethyl 4-methoxybenzoate	5.6
Ethyl 4-dimethylaminobenzoate	6.3
Methyl trichloroacetate	3.3
Ethyl triflouroacetate	3.2
Ethyl trichloroacetate	3.4
Ethyl 4-nitrobenzoate	4.5
Ethyl 4-cyanobenzoate	5.1
Diethyl terephthalate	4.8
Isopropyl ethanoate	5.6
Ethyl 2,2-dimethylpropanoate	5.4
Ethyl phenylacetate	5.4
Ethyl 1-adamantanecarboxylate	5.4
Ethyl ethanoate	5.4
Ethyl propionate	5.5
tert-Butyl ethanoate	5.5
12-Crown-4	5.6
15-Crown-5	5.6
Dipentyl ether	5.4
n-Propylethylether	5.2
Dimethyl ether	5.1
Dipropyl ether	5.2
Diphenyl ether	3.1
Anisole	3.3
1,4-Thioxane	4.7
Trimethoxy orthoformate	4.3
Dimethoxymethane	4.4
Tetramethyl orthocarbonate	5.0
Hexamethyldisiloxane	1.9
tert-Butyl methyl ether	5.7
Dibenzyl ether	4.5
2-Chloroethyl ethyl ether	4.0
Ethyl vinyl ether	3.3
Bis(2-Chloroethyl) ether	3.0
Dichloromethyl methyl ether	2.9
1,1,1,3,3,3-Hexafluoro-isopropyl methyl ether	2.2
Diisopropyl ether	5.5
1,2-Diethoxyethane	5.5
tert-Butyl ethyl ether	5.5
1,2-Dimethoxyethane	5.3
Diethyl ether	5.3
Dibutyl ether	5.0
Di-tert-butyl ether	4.7
Diallyl ether	4.6
2,3-diadamant-2-yl oxirane	6.3
1,4-Dioxane	4.7
1,3-Dioxane	4.5
2,3-Dihydrofuran	4.2
1,3-Dioxolane	4.1
Epichlorhydrin	4.0
3,4-Dihydro-2H-pyran	4.0

1,3,5-Trioxane	3.1
Furan	2.2
2,2,5,5-Tetramethyltetrahyrdofuran	6.2
Cineole	6.1
Triethylene oxide	6.1
2-Methyltetrahydrofuran	6.0
Tetrahydrofuran	5.9
Tetrahydropyran	5.8
Cyclohexene oxide	5.6
Propylene oxide	5.2
Chloroform	0.8
2-Bromo-2-methylpropane	2.3
Chlorobenzene	1.8
Bromobenzene	1.4
Fluorobenzene	1.6
Tetrachloromethane	0.6
1,3-Difluoropropane	2.5
1,3-Dichloropropane	1.9
1,4-Dichlorobutane	2.0
1-Chlorobutane	2.2
1,5-Dichloropentane	2.2
1-Chloropentane	2.2
2-Chloropropane	2.4
Chlorocyclohexane	2.5
2-Chloro-2-methylpropane	2.4
1-Chloroadamantane	2.7
1-Fluoropentane	2.9
1-Fluorooctane	3.1
Fluorocyclohexane	3.3
1-Fluoroadamantane	3.6
1,1,1-Trichloroethane	1.5
Dichloromethane	2.0
1,1-Dichloroethane	1.5
1,2-Dichloroethane	2.4
Dibromomethane	1.5
2-Bromopropane	2.4
Bromocyclohexane	2.5
1-Bromoadamantane	2.7
1,2-Dibromoethane	1.7
1,3-Dibromopropane	1.9
Bromocyclopropane	2.0
1,4-Dibromobutane	2.0
Bromoethane	2.2
1-Bromopropane	2.2
1-Bromopentane	2.3
1-Bromobutane	2.3
Ascaridole	5.1
3,4-diadamantyl-2-yl-dioxetan	4.5
tert-Butyl peroxide	3.4
3-Methylphenol	3.1
3-Trifluoromethylphenol	2.3
4-Methylphenol	3.1

4-Fluorophenol	2.8
Phenol	2.9
Pentafluorophenol	0.8
Triphenyl phosphine	5.5
Dibutyl selenide	3.5
Diethyl selenide	3.4
Tributylphosphine sulphide	6.3
Trioctylphosphine sulphide	6.5
O-methyl dimethylthiocarbamate	4.9
Methimazole	8.1
ε-Thiocaprolactam	6.6
N,N-Dimethyl(N,N-dimethylamino)methyl-ideneaminothioamide	7.0
N,N-Dimethyl-1-(N,N-dimethylamino)-ethylideneaminothioamide	7.6
N,N-Dimethylthiobenzamide	5.3
N,N-Dimethylthioformamide	5.4
N-Methylthioacetamide	5.6
4,N,N-Trimethylthiobenzamide	5.6
N,N-Dimethyl-4-methoxythiobenzamide	5.6
N,N-Dimethylthioacetamide	6.0
N,N-Dimethyl-4-aminothiobenzamide	6.0
methyl dimethylthiocarbamate	4.5
Oxazolidine-2-thione	6.1
3-Methylthioazole-2(3H)-thione	4.9
1,3-Dimethylimidazol-2(3H)-thione	6.5
3-Methylthiazolidine-2-thione	5.1
3,4,5-Trimethyloxazole-2(3H)-thione	5.8
3,4,5-Trimethylthioazole-2(3H)-thione	5.6
1,3,4,5-Tetramethylimidazole-2(3H)-thione	7.0
Benzo[d]3-methyloxazole-2(3H)-thione	4.8
Benzo[d]3-methyloxazole-2(3H)-thione	4.5
Benzo[d]1,3-dimethylimidazole-2(3H)-thione	5.7
Thiazolidine-2-thione	6.0
4,5-Dimethyloxazole-2(3H)-thione	7.1
4,5-Dimethylthiazole-2(3H)-thione	7.1
1,4,5-Trimethylimidazole-2(1H)-thione	7.9
Benzo[d]oxazole-2(3H)-thione	5.8
Benzo[d]thiazole-2(3H)-thione	5.6
Benzo[d]imidazole-2(3H)-thione	6.5
Ethyl isothiocyanate	2.9
Ethylenetrithiocarbonate	3.7
Thiocamphor	3.8
N,N-Dimethylthiocarmomyl chloride	4.2
Dihydro-2(3H)-thiophenone	5.2
Diethyl sulphide	3.6
Thiophene	2.2
Ethyl methyl sulphide	3.1
Dibutyl sulphide	3.6
Di(tert-butyl) sulphide	3.6
Tetrahydrothiophene	3.3
Dimethyl sulphide	3.5

Diisopropyl sulphide	3.8
Isobuty n-butyl sulphide	3.5
Sec-butyl n-butyl sulphide	3.6
tert-butyl n-butyl sulphide	3.7
Triethyl thiophosphate	4.7
Hexamethylthiophosphoramide	6.0
1-Methylimidazolidine-2-thione	7.2
N,N-Dimethyl-N',N'-diethylthiourea	5.9
N,N'-Dimethyl-N,N'-ethylenethiourea	6.0
N,N,N',N'-Tetramethylthiourea	6.1
N-Methyl-N,N'-propylenethiourea	7.5
Pyridine N-oxide	9.0
Trimethyl phosphate	8.5
Triethyl phosphate	8.8
Tributyl phosphate	8.6
Triphenyl phosphate	7.0
Trimethylphosphine oxide	10.7
Triphenylphosphine oxide	10.1
Tripropylphosphine oxide	10.8
Tributylphosphine oxide	10.2
Triethylphosphine oxide	10.1
Diethyl phosphite	8.3
Dimethyl phosphite	8.0
Diisopropyl phosphite	8.6
Diethyl isopropylphosphonate	9.1
Di-(1-chloropropyl) methylphosphonate	8.7
Diethyl chloromethylphosphonate	8.5
Diethyl dichloromethylphosphonate	7.8
Diethyl trichloromethylphosphonate	7.3
Dimethyl ethylphosphonate	9.0
Diethyl methylphosphonate	9.1
Diethyl ethylphosphonate	9.2
Hexamethylphosphoramide	10.9
N1,N1-Dimethyl-N2-cyanoacetamidine	8.0
cyanamide	5.6
dimethylcyanamide	6.5
1-piperidinecarbonitrile	6.6
diethylcyanamide	6.7
N1,N1-dimethyl-N2-cyanoformamidine	7.7
Methyl thiocyanate	4.7
Ethyl thiocyanate	4.4
Diphenylphosphinous cyanide	4.8
Cyanogen Bromide	3.5
Trimethylammonioacetamidate	10.3
Trimethylsillylcyanide	5.1
N'-cyano-N-methyl-N-propylguanidine	7.9
Chloroacetonitrille	3.9
isobutylnitrile	5.3
4-methoxybenzonitrile	5.2
trimethylacetonitrile	5.3
4-dimethylaminobenzonitrile	5.8
trans-3-dimethylaminoacrylonitrile	6.8

4-Chlorobenzonitrille	4.5
acrylonitrile	4.6
benzonitrile	4.8
2,6-dimethylbenzonitrile	5.0
allylcyanide	5.0
acetonitrile	5.1
propionitrile	5.2
N,N-Dimethylamino(thioxo)acetonitrille	4.4
Pentafluorobenzonitrille	3.1
1-Cyanopentane	5.2
Dichloroacetonitrille	3.4
1-Cyanobutane	5.2
Trichloroacetonitrille	2.3
Phenylacetonitrille	4.8
Cyanoacetylene	3.7
4-fluorobenzonitrille	4.7
Phenylcyanate	4.8
3-Toluonitrille	5.0
Cyclopropylcyanide	5.4
Methoxyacetontrille	4.7
1-Methoxy-2-cyanoethane	5.1
N,N-Dimethyl-N-nitrosoamine	5.8
N,N-Diphenyl-N-nitrosoamine	4.3
Nitromethane	3.7
Nitrobenzene	3.7
N-Nitrocamphorimine	3.8
2-Nitropropane	4.0
4-Nitro-o-xylene	4.1
4-Nitroanisole	4.2
N,N-Diethyl-4-nitroaniline	5.1
1-Dimethylamino-2-nitroethylene	6.3
1-Piperidino-2-nitroethylene	6.5
Nitroethane	3.8
2-Methyl-2-nitropropane	4.0
4-Nitrotoluene	3.8
4-Chloronitrobenzene	3.6
3-Chloronitrobenzene	3.4
Dimethyl carbonate	4.9
Proplyene carbonate	5.8
Ethyl methyl carbonate	4.9
Diethyl carbonate	5.0
Vinylene carbonate	4.6
Diethyl sulphate	4.8
Diethyl sulphite	4.9
N-Methylmethanesulphonamide	5.9
N,N-Dimethyltoluene-p-sulphonamide	6.2
N,N-Dimethyltoluene-p-sulphonamide	7.7
N,N-dimethylbenzenesulfinamide	7.6
N-Methyl,N-Benzylsulfonamide	6.1
N,N-Dimethyl-N'-phenylsulfonylformamidine	7.1
N-(p-Tolysulfonylimino(dimethyl)-λ4-sulfane)	7.8
N-Trimethylammoniotoluene-p-sulfonamidate	8.9

N-Trimethylammoniooctanesulfonamidate	9.5
N,N-Dimethylbenzenesulphonamide	5.7
N,N-Dimethylmethanesulphonamide	6.0
N,N,N',N'-Tetraethylsulfamide	6.3
N,N-Dimethylmethanesulphinamide	8.2
Ethyl methanesulphonate	5.3
Diphenyl sulphone	5.9
Diphenyl sulphone	5.8
Dimethyl sulphone	6.2
Tetramethylene sulfone	6.3
Dibutyl sulphone	6.4
Dimethyl sulphoxide	8.6
Di-isopropyl sulphoxide	8.7
Dibutyl sulphoxide	8.7
Diphenyl sulphoxide	7.5
Di(p-tolyl) sulphoxide	7.8
Tetrahydrothiophene S-oxide	8.6
(methylsulfinyl)benzene	7.8
2-Aminopyrimidine	7.2
2-Methylaminopyridine	7.7
2-N,N-Dimethylaminopyridine	6.6
2,2'-Bipyridine	5.6
4-N,N-Dimethylaminopyridine	9.3
Acridine	7.4
4-(N,N-Dimethylamino)quinoline	8.5
2-Aminopyridine	7.8
Phenazine	6.0
2-(N,N-Dimethylamino)pyrimidine	6.2
4-Pyrrolidinopyridine	9.6
7,8-Benzoquinoline	5.6
Thiazole	7.3
2,6-Dimethylpyridine	7.8
2,4,6-Trimethylpyridine	8.1
1,7-Phenanthroline	7.2
3-(N,N-Dimethylamino)pyridine	8.5
Phenanthridine	7.2
4-Piperidinopyridine	9.0
4-(4-Methylpiperidino)pyridine	9.0
5-(N,N-Dimethylamino)pyrimidine	7.2
Quinoline	7.3
4-N,N-Diethylaminopyridine	9.5
N-Methyl-N-pyridin-4-ylhydrazine	8.8
2-Methylpyridine	7.6
4-Chloropyridine	6.5
4-Cyanopyridine	5.4
3-Aminopyridine	7.9
Quinazoline	6.5
3,5-Dimethylpyridine	8.0
4-methylaminopyridine	9.0
3,4-Dimethylpyridine	8.0
2-Ethylpyridine	7.4
2-Vinylpyridine	6.7

4-Acetylpyridine	6.4
3-Benzoylpyridine	6.4
Isoquinoline	7.4
Benzothiazole	6.1
2,5-dimethylpyrazine	5.9
4-Vinylpyridine	7.4
1-methylpyrazole	7.1
1-Butyl-1,3,4-triazole	10.5
2-Isopropylpyridine	7.0
3-Cyanopyridine	5.3
2-Butylpyridine	7.2
3,5-Dichloropyridine	5.0
4-Phenylpyridine	7.4
3-Chloropyridine	6.0
3-Methylpyridine	7.5
3-Bromopyridine	6.0
3-Ethylpyridine	7.5
4-Methylpyridine	7.7
Methyl nicotinate	6.4
2-Phenylpyridine	6.2
4-tert-Butylpyridine	7.7
Pyridine	7.2
4-Ethylpyridine	7.7
4-Methoxypyridine	7.8
2-Methoxypyridine	5.3
4-Aminopyridine	8.7
3-Fluoropyridine	6.1
4,6-dimethylpyrimidine	6.3
2,4,5-trimethyloxazole	7.5
4-(N,N-Dimethylamino)pyrimidine	7.7
2-tert-Butylpyridine	6.2
5-bromo-1-methylimidazole	8.0
2,4-Dimethylpyridine	7.2
4-Isopropylpyridine	7.4
4-methylimidazole	8.9
Pyrazine	5.1
9-(N,N-Dimethylamino)acridine	8.2
2,6-Diethylpyridine	6.6
2,5-dimethyl 1,3,4 thioazole	7.2
1-Phenylethyl-1,2,3-triazole	8.7
5-Bromopyrimidine	4.4
Pyrimidine	5.4
3-N,N-Diethylcarbomylpyridine	7.7
1-methylimidazole	9.1
2-Cyanopyridine	5.0
2-Thiobenzoimidazole	4.2
2-methylsulfide-5-methyl-1,3,4-thioazole	6.3
Imidazole	8.5
1-Benzyl-1,2,4-triazole	7.0
2-Bromopyridine	5.4
2-Chloropyridine	5.4
s-Triazine	3.8

Oxazole	5.8
2,5-diphenyl 1,3,5 oxazole	3.8
Phtalazine	7.4
1-Methylbenzotriazole	6.6
Pyridazine	6.7
2-Fluoropyridine	5.2
Pentafluoropyridine	2.0
2-Methyl-1-pyrroline	8.8
Tetramethylguanidine	10.2
N,N-dimethylimidoformamide	10.0
(1E)-Cyclohex-3-en-1-one O-decyloxime	5.5
Acetone O-phenyloxime	4.8
Isoxazole	4.7
2,6-Difluoropyridine	3.4
2,6-di-tert-butylpyridine	1.9
10,11-dihydro-5H-tetrazolo[1,5-b][2]benzazepine	6.3
3,5-difluorobenzylamine	5.9
3-flourobenzylamine	6.6
3-methylbenzylamine	7.4
Pentylamine	7.8
Hexylamine	7.7
Heptylamine	7.7
Nonylamine	7.9
Decylamine	7.8
Octadecylamine	8.1
Ethylenediamine	8.7
2-Methoxyethylamine	8.1
3-Methoxypropylamine	8.1
ethylamine	7.9
tert-butylamine	8.1
benzylamine	7.2
Adamantan-1-amine	8.2
1,3-Diaminopropane	8.9
1,4-Diaminobutane	8.0
1,6-Diaminohexane	8.0
Phenethylamine	7.9
Allylamine	7.4
Propargylamine	6.6
Aminopropionitrile	5.9
2,2,2-Trifluoroethylamine	4.6
c-Hexylamine	8.1
n-Hexadecylamine	8.1
Isopropylamine	8.0
n-Butylamine	8.0
n-Propylamine	7.9
c-Propylamine	6.9
n-octylamine	8.1
2-Dimethylamino-3,3-dimethylazirine	8.6
Ammonia	6.8
Methylamine	7.8
1,2,3,6-tetrahyrdopyridine	7.9
dimethylamine	8.1

N-methylethylamine	8.1
piperidine	8.3
pyrrolidine	8.8
azetidine	8.8
Morpholine	7.2
Dipropylamine	7.9
Dibutylamine	7.9
Dipentylamine	7.9
Diethylamine	7.9
Di-isopropylamine	7.5
Dibenzylamine	6.3
1,2,2,6,6-pentamethylpiperidine	5.8
N,N'-dimethylpiperazine	7.2
hexamethylenetetramine	6.0
N,N-dimethylpropargylamine	6.6
N,N-dimethylallylamine	7.3
3-chloroquinuclidine	7.4
1-methyl-1,2,3,6-tetrahydropyridine	7.5
N-methylpiperidine	7.7
trimethylamine	7.8
N,N-dimethylethylamine	7.9
N-methylpyrrolidine	7.9
quinuclidine	9.1
N,N-dimethylbenzylamine	6.6
Nicotine	7.7
N-Methylmorpholine	6.9
1,4-Diazabicyclo[2.2.2]octane	8.9
Triphenylamine	3.6
N-(4-Nitrobenzyl)piperidine	6.9
N,N-dimethyl-N-[(E)-2-phenylvinyl]amine	7.3
Tribenzylamine	3.8
Cyclohexyldimethylamine	7.8
Triethylamine	7.5
Tripropylamine	6.6
Tributylamine	6.8
Tripentylamine	6.9
Trioctylamine	7.0
Triallylamine	6.1
Aniline	4.5
4-Bromoaniline	4.1
2-Methylaniline	4.5
4-Methylaniline	4.9
3-Methylaniline	4.7
N,N-Dimethylaniline	4.2
N,N-Diethylaniline	4.9
3-Fluoroaniline	3.7
4-Fluoroaniline	4.3
3-Chloroaniline	3.6
4-Chloroaniline	4.1
3-Bromoaniline	3.4
3-Iodoaniline	3.6
4-Iodoaniline	3.8

3-Methoxyaniline	4.7
4-Methoxyaniline	5.3
Diphenylaniline	3.2

Table S2. H-bond donor parameters.

Compound Name	***α***
Water	2.8
Butan-1-ol	2.7
Di-tert-butylmethanol	2.5
3-Isopropyl-2,2,4,4-tetramethylpentan-3-ol	2.2
2,2,2-Trichloroethanol	3.4
2,2,2-Tribromoethanol	3.3
2,2,3,3-Tetrafluoropropan-1-ol	3.5
Trimethylsilanol	3.0
N,N-Dibenzylhydroxylamine	3.2
N,O-Dibenzylhydroxylamine	2.9
Neopentanol	2.7
1,1,1,3,3,3-Hexafluoro-2-trichloromethylpropan-2-ol	4.4
tert-Pentanol	2.6
2-Fluoroethanol	3.0
Hexachloropropan-2-ol	4.0
Benzyl alcohol	3.0
Pentafluorobenzyl alcohol	3.3
1,1,1-Trichloro-2-methylpropan-2-ol	3.0
1,1,1-Trifluoro-2-methylpropan-2-ol	3.3
1,1,1,3,3,3-Hexafluoro-2-methylpropan-2ol	4.0
Butyl sulphide	1.3
Cyanic acid	3.6
(E)-2,2-Dimethyl hexan-1-phenyl hydroxylamine	3.1
4a-phenyloctahydronaphthalen-2(1)-one oxime	3.0
3-Ethyl-2,4-dimethylpentan-3-ol	2.4
2,2,2-Trifluoroethanol	3.7
Hexafluoropropan-2-ol	4.5
Methanol	2.9
Ethanol	2.7
Propan-1-ol	2.6
Hexan-1-ol	2.7
Propan-2-ol	2.7
tert-Butyl alcohol	2.7
2-Chloroethanol	3.3
Butan-2-ol	2.5
Cyclohexanol	2.6
Cholesterol	2.6
2,2,2-Trifluoro-1,1-bis(triflouromethyl)ethanol	4.9
3-chloro-3-methylbut-1-yne	2.0
tert-Butylethyne	1.9
Benzoylethyne	2.1
Diethyl prop-2-ynyl phosphate	2.2
Pentylacetylene	1.9
Phenylacetylene	2.0
Thioethylacetylene	2.1
4-bromophenylacetylene	2.1
Chloromethylacetylene	2.1
Bromomethylacetylene	2.1
4-nitrophenylacetylene	2.1
Trifluoromethylacetlyene	2.5

Cyanoacetylene	2.8
But-3-yn-2-one	2.3
Triethylsilylacetylene	2.0
Ethyl ethynyl ether	1.9
Ethyl propiolate	2.3
Succinimide	3.4
N-Phenylurethane	2.8
Acetanilide	3.3
4-(Diethylamino)acetanilide	2.7
3-Chloro-4-nitroacetanilide	4.2
3-(Trifluoromethyl)-4-nitroacetanilide	4.2
1-oxa-2-azaspiro[4,5]decan-3-one	3.1
Trifluoroacetamide	3.4
N-hexylheptamide	2.8
N-Methylacetamide	2.9
Maleimide	3.4
N,N-hexafluorodiethamide	4.3
2-Ethyl-2-methylsuccinimide	3.4
2-methyl-3-chloromaleimide	3.6
2,3-Dichloro-3-methylmaleimide	4.1
Tetrafluorosuccinimide	5.0
N-Methylformamide	2.9
Trifluorobenzoacetamide	3.9
Ammonia	2.2
N-Nitromethylamine	3.8
N-Nitropropylamine	3.7
N-Nitrobutylamine	3.7
N-Cyclohexylamine	3.6
N,3,3,3-Tetranitropropylamine	4.5
α-Naphthylamine	2.6
β-Naphthylamine	2.8
1,2,3,4-Tetrahydroquinoline	2.8
10,11-dihydro-5H-dibenzo[b,f]azepine	2.8
5-Nitroindoline	3.1
N-Methyl-tert-butamide	2.9
2-Chloro-4-nitroaniline	3.2
4-Chloro-2-nitroaniline	3.2
Diphenylaniline	2.7
2-Nitroaniline	2.9
3-Nitroaniline	3.0
4-Nitroaniline	3.1
4-Bromoaniline	2.6
N-Methylaniline	2.1
4-Nitro-N-Methylaniline	3.0
Aniline	2.4
Trifluoroacetic acid	5.3
Trichloroacetic acid	5.2
Pentafluorobenzoic acid	5.0
2-Bromobenzoic acid	4.0
Chloroacetic acid	4.7
Hexanoic acid	3.3
tert-Butanoic acid	3.5

Acetic acid	3.6
Dichloroacetic acid	5.0
Benzoic acid	4.2
1,1,1-Trichloroethane	1.4
Dichloromethane	1.9
1,2-Dichloroethane	1.7
Bromoform	2.1
2,2-Dichloro-1,1-difluoroethyl methyl ether	2.0
2-Chloro-1,1,2-difluoroethyl difluoromethyl ether	2.1
1,2-Dichloro-1,2-difluoroethane	2.2
Bromodichloromethane	1.9
1,2-Dibromo-1,1-difluoroethane	1.9
1,2-Dichloro-1-fluoroethane	2.1
1-Chloro-1,1,2-trifluoro-2-iodoethane	2.1
1,1,2-Trichloro-2,2-dfluoroethane	2.2
1-Bromo-2-chloro-1,1,2-trifluoroethane	2.2
1-Bromo-1-chloro-2,2,2-trifluoroethane	2.3
Chloroform	2.2
3-(1H-imidazol-2-yl)propyl phenyl carbanoate	3.4
Tetrachloropyrrole	4.3
Tetrabromopyrrole	4.2
Tetraiodopyrrole	3.8
Indole	3.1
5-Fluoroindole	3.3
Carbazole	3.3
4-Aminopyrimidine	2.9
5-Aminopyrimidine	2.9
3-Aminopyridine	2.8
2-Aminopyridine	2.7
4-Aminopyridine	3.0
2-Aminopyrimidine	2.7
Propyl-2-imidazole benzoate	3.2
3-Triazolepropylphenyl	3.8
3-Methylthio-1,2,3-Triazole	3.9
4-Trifluoromethane-1,2,3-triazole	4.3
5-Phenyl-1,2,3,4-tetrazole	5.0
2-Aminobenzothiazole	3.1
Pyrrole	3.0
3-methylpyrazole	3.6
5-methylpyrazole	3.6
3,5-dimethylpyrazole	3.6
3,4,5-trimethylpyrazole	3.4
pyrazole	3.6
4-methylpyrazole	3.5
4-Bromopyrazole	3.9
3,5-Dimethyl-4-bromopyrazole	3.9
1,1-Dintroethane	3.0
Ethyl N-Nitrocarbamate	3.9
4-Chloroperoxybenzoic acid	2.9
3-Chloroperoxybenzoic acid	2.9
4-tert-Butylperbenzoic acid	2.6
2-Methoxyphenol	2.4

2-Methylphenol	3.5
2-Isopropylphenol	3.6
2-tert-Butylphenol	3.4
3-Methylphenol	3.7
3-Fluorophenol	4.1
3-Chlorophenol	4.2
3-Bromophenol	4.2
3-Trifluoromethylphenol	4.3
3-Nitrophenol	4.6
4-Methoxyphenol	3.7
4-Methylphenol	3.7
4-sec-Butylphenol	3.7
4-tert-Butylphenol	3.6
4-Fluorophenol	3.9
Phenol	3.8
4-Chlorophenol	4.1
3,4-Dichlorophenol	4.4
3,5-Dichlorophenol	4.5
3,5,6-Trichlorophenol	4.7
Pentafluorophenol	4.5
Pentachlorophenol	3.6
Pentabromophenol	3.4
1-Naphthol	3.8
2-Naphthol	3.9
4-Bromophenol	4.1
4-Iodophenol	4.1
4-Acetylphenol	4.3
4-Cyanophenol	4.6
3,4-Dimethylphenol	3.6
2-Methyl-6-tertbutylphenol	2.9
3-Ethylphenol	3.6
3-Dimethylaminophenol	3.5
3-Methoxyphenol	3.8
3-Cyanophenol	4.5
4-Ethylphenol	3.6
4-Propylphenol	3.6
4-Isopropylphenol	3.6
4-Octylphenol	3.6
4-Phenylphenol	3.8
4-Trifluoromethylphenol	4.3
2,3-Dimethylphenol	3.5
2,4-Dimethylphenol	3.5
2,5-Dimethylphenol	3.6
3,4,5-Trimethylphenol	3.6
4-Bromo-2,6-dimethylphenol	3.3
2,6-Dichloro-4-nitrophenol	4.2
3,5-Dimethylphenol	3.7
4-Methyl-2-tert-butylphenol	3.7
3-Methyl-6-tert-butylphenol	3.6
2,4-di-tert-butylphenol	3.6
4-Nitro-3-trifluoromethylphenol	5.3
3,5-Di(trifluoromethyl)phenol	4.7

2,3,5-Trimethylphenol	3.5
α-Heptafluoronaphthol	4.1
β-Heptafluoronaphthol	4.5
2-Chlorophenol	4.0
3-Isopropylphenol	3.7
4-Nitrophenol	4.7
2,6-Dimethylphenol	3.3
2-Cyanophenol	4.7
2,6-Dichlorophenol	3.2
3-methylmethanoate phenol	4.2
2,4,6-Trimethylphenol	3.0
2,6-Diisopropylphenol	2.8
N,N,N',N'-Tetramethyl-N''-benzyl-N''-prop-2-ynylphosphoric triamide	1.9
Prop-2-ynyl bis(piperidino)phosphinate	1.9
Prop-2-ynyl bis(diethylamido)phosphinate	1.9
Prop-2-ynyl bis(dimethylamido)phosphinate	2.0
But-3-ynyl bis(dimethylamido)phosphinate	1.9
Prop-2-ynyl bis(dibutylamido)phosphinate	2.0
N''Ethyl-N,N,N',N'tetramethyl-N''-prop-2-ynyl-phosphoric triamide	1.8
Prop-ynyl bis(morpholino)phosphinate	2.1
Pentamethyl(prop-2-ynyl)phophoric triamide	1.9
Touluene-p-sulfonamide	3.2
N-Benzyltoluene-p-sulfonamide	3.0
N-(2-Naphthyl)toluene-p-sulfonamide	3.2
Thioacetamide	3.7
Thioacetanilide	3.4
Isopropyl sulphide	1.3
t-Butyl sulphide	1.3
Thiocyanic acid	4.4
Ethyl sulphide	1.4
Propyl sulphide	1.4
Thiophenol	1.7
O-Prop-2-ynyl bis(dimethylamido)thiophosphinate	2.0
S-Prop-2-ynyl bis(dimethylamido)thiophosphinate	2.1
Thiazolidin-2-one	3.6
Oxazolidin-2-one	3.4
4,5-Dimethyloxazol-2(3H)-one	4.0
4-Methylthiazol-2(3H)-one	4.1
Benzo[d]oxazol-2(3H)-one	4.4
Benzo[d]thiazol-2(3H)-one	4.3
1-Methylbenzo[d]imidazol-2(1H)-one	3.9
1-Methylimidazolidin-2-one	3.2
5-Methyl-4-tert-butylthiazole-2(3H)-one	3.2
N-Methyl-N,N'-propylenethiourea	3.0
1-Methylimidazolidine-2-thione	3.3
Oxazolidine-2-thione	4.1
Thiazolidine-2-thione	3.6
4,5-Dimethyloxazole-2(3H)-thione	4.3
4,5-Dimethylthiazole-2(3H)-thione	4.3
1,4,5-Trimethylimidazole-2(1H)-thione	3.9

Benzo[d]oxazole-2(3H)-thione	4.6
Benzo[d]thiazole-2(3H)-thione	4.5
Thiazolidine-2-selone	3.9
Benzo[d]imidazole-2(1H)-thione	4.0
3-Methyl-1,2,4-thiadiazole-5(4H)-thione	4.9
3-Phenyl-1,2,4-thiadiazole-5(4H)-thione	4.9
1,3-Dimethyl-1,2,4-triazole-5(4H)-thione	4.5
4-Phenylthiazole-2(3H)-thione	4.3
Thiazole-2(3H)-thione	4.0
4-Methylthiazole-2(3H)-thione	3.9
4-Ethylthioazole-2(3H)-thione	3.9
4-Isopropylthiazole-2(3H)-thione	3.8
4-tert-Butylthiazole-2(3H)-thione	3.8
4-Ethyl-5-methylthiazole-2(3H)-thione	3.8
4-Isopropyl-5-methylthiazole-2(3H)-thione	3.6

Table S3. Phase transfer free energies in kJ mol^{-1}.

	$\Delta G_{w\to l}$		$\Delta G_{l\to w}$		$\Delta G_{l\to h}$		$\Delta G_{o\to w}$		$\Delta G_{h\to w}$	
solvent	**expt**	**calc**	**expt**	**calc**	**expt**	**calc**	**expt**	**calc**	**expt**	**calc**
tetramethylsilane		17.9	30.8	31.4	-1.1	0.3	23.9	30.4	31.9	31.1
n-pentane	19.0	19.3	28.7	27.4	-0.4	-0.2	24.7	26.5	29.0	27.5
2-methylbutane	19.5	19.2	28.1	28.1		0.0		27.0		28.1
n-hexane	18.7	19.5	31.9	31.6	-0.3	-0.2	27.6	30.5	32.6	31.8
cyclohexane	20.5	19.5	26.7	27.9	-0.6	-0.3	25.0	27.0	28.7	28.2
n-heptane	18.8	19.5	35.4	35.3	-0.2	-0.3	32.0	34.1	36.2	35.5
n-octane	18.4	19.5	39.7	39.0	-0.2	-0.3	34.8	37.8	40.0	39.3
2,2,4-trimethylpentane	19.7	19.3	36.7	37.5	-0.1	-0.3	38.7	36.4	36.6	37.9
n-decane	18.5	19.5	49.8	51.1		0.3	43.6	48.6		50.8
n-dodecane	18.4	19.6		59.0		0.1		56.3		58.8
n-hexadecane	18.1	19.5		73.6	1.5	-0.3		70.8		73.8
benzene	14.6	15.4	19.3	19.6	0.1	0.5	17.5	19.0	19.2	19.1
toluene	15.8	15.3	22.8	22.9	0.0	0.6	20.9	22.0	22.7	22.2
o-xylene	14.8	15.5	25.9	26.8	0.2	0.7	23.3	25.7	25.6	26.1
m-xylene	15.0	15.2	26.3	25.8	0.1	0.7	23.7	24.8	26.0	25.0
p-xylene	14.7	15.5	26.1	26.1	0.0	0.6	23.4	25.2	25.9	25.5
ethylbenzene	14.8	15.8	26.2	26.7	0.3	0.5	23.4	25.8	25.6	26.2
isopropylbenzene	15.4	16.3	28.6	31.4		0.4	26.3	30.3	28.4	31.0
1,3,5-trimethylbenzene	15.5	15.5	29.4	29.3		0.7	24.9	28.3	29.2	28.6
styrene	13.8	15.3	24.4	23.7		0.5	23.4	23.2		23.2
tetralin		15.9	26.2	30.0		0.3	25.3	29.2		29.7
cis-decalin	17.7	19.6	39.6	37.0		-0.9		36.4		37.9
water	0.0	0.0	0.0	0.0	18.0	19.5	3.2	-6.2	-18.0	-19.5
methanol		1.5	1.0	1.4	10.2	11.7	1.2	-1.3	-9.2	-10.3
ethanol	5.2	2.8	0.6	3.8	8.8	10.5	3.7	2.0	-5.5	-6.7
1-propanol		3.7	6.4	6.9	7.9	9.8	6.8	5.7	-1.4	-2.9
2-propanol		3.7	7.5	6.8	7.6	10.0	5.7	5.1	-2.6	-3.3
1-butanol	1.6	4.4	9.8	10.0	8.0	9.5	10.1	9.1	2.0	0.5
2-methyl-1-propanol	1.9	6.0	9.1	12.3	4.4	8.4	9.7	11.7	1.8	3.9
2-butanol	0.7	5.9	8.4	12.0	6.8	8.0	9.0	11.4	0.9	4.0
2-methyl-2-propanol		4.3	6.2	10.3	6.6	9.2	7.4	8.9	-0.3	1.0
1-pentanol	3.1	5.2	13.4	13.6	7.5	8.5	14.1	13.2	5.5	5.1
3-methyl-1-butanol	2.7	5.3	12.9	14.3	9.0	8.7	12.7	13.7	3.8	5.7
2-methyl-2-butanol	1.3	5.2	9.2	11.0	5.9	7.9	10.5	10.7	3.6	3.1
1-hexanol	2.9	5.6	16.6	17.1	7.3	8.1	17.0	17.0	9.1	9.0
cyclohexanol	2.1	5.0	12.3	13.4	7.4	8.5	12.4	12.8	5.0	4.9
1-octanol	3.2	6.2	24.9	23.4	7.7	7.5	22.5	23.8	16.2	16.0
1-decanol	3.5	7.5	30.7	35.4	6.9	7.5	31.5	35.2	23.8	28.0
1-dodecanol	5.6	8.0	36.4	42.6		7.0	34.7	42.5		35.6
benzyl alcohol	2.6	7.2	12.2	14.3	7.5	8.8	11.4	14.6	5.7	5.5
2-phenylethanol	6.5	6.7	14.0	16.2		8.6	13.1	16.0		7.6
allyl alcohol		3.9	5.0	4.9	7.9	9.4	6.4	3.3	-2.8	-4.5
2-chloroethanol		4.8		8.5		8.6	5.0	10.6		0.0
2-cyanoethanol		5.3		7.0		13.7	0.0	7.4		-6.7
2,2,2-trifluoroethanol		3.9	5.6	5.0	9.7	11.3	7.4	7.6	-4.1	-6.3
1,1,1,3,3,3-hexafluoro-2-propanol		0.2	6.0	7.7		5.1	14.9	18.8		2.7
2-methoxyethanol		3.2	0.4	1.2		12.0	1.0	-0.6		-10.9
2-ethoxyethanol		4.2		4.4		11.0	3.8	3.2		-6.6
ethylene glycol		1.9	1.4	-0.8	21.7	21.9	-2.4	-5.5	-20.3	-22.6

1,2-propanediol		3.1		2.7		19.5	0.1	-0.6		-16.8
1,3-propanediol		1.2		-2.5		21.5	-0.6	-6.0		-24.0
1,2-butanediol		4.1		6.1		17.5		3.8		-11.4
2R,3S-butanediol		4.1		3.3		16.6		1.6		-13.3
1,4-butanediol		2.3		1.8		21.4	0.6	-2.2		-19.6
1,5-pentanediol		2.5		3.5		20.0	2.9	0.8		-16.4
diethylene glycol		3.4		1.9		20.7	-5.9	-0.8		-18.8
triethylene glycol		4.3		7.5		20.5	-1.5	5.5		-13.0
glycerol		3.1		1.5		22.7	-4.7	-3.1		-21.2
phenol	1.0	5.0	10.0	11.4	7.6	7.9	13.9	15.3	2.7	3.5
o-cresol		5.3	13.0	15.5	6.1	6.2	16.7	20.3	6.6	9.3
m-cresol	1.8	5.9	13.5	14.4	7.5	7.8	16.7	18.1	8.6	6.5
p-cresol		5.9	13.8	14.0	7.9	7.7	16.6	17.6	5.9	6.3
2,6-dimethoxyphenol		8.2	14.0	16.7		5.9	11.9	16.3		10.8
6-amino-2,4-dimethylphenol		6.4	16.7	18.3		5.9	18.7	22.8		12.4
3-chlorophenol	1.2	1.3	13.6	13.4		6.1	19.7	22.0		7.2
diethyl ether	7.1	3.8	10.4	9.5	0.1	1.3	10.5	10.4	12.0	8.2
di-n-propyl ether	9.1	5.2	17.5	21.0	0.0	1.3	17.0	21.3	19.1	19.7
di-i-propyl ether	8.6	3.8	15.2	16.6	0.4	1.2	14.1	17.9	19.3	15.4
di-n-butyl ether	10.7	6.1	25.0	28.2	-0.3	1.2	23.7	28.4	26.3	27.0
bis(2-chloroethyl) ether	12.0	14.2	16.5	25.7		2.0	12.7	25.1		23.7
1,2-dimethyoxyethane		4.0	3.6	2.9	1.7	3.0	4.2	3.0	1.9	-0.1
diethylene glycol dimethyl ether		5.5		12.1		3.6	3.3	11.4		8.5
furan	11.2	13.0	14.7	14.5		1.2	13.0	13.9		13.3
tetrahydrofuran		-1.3	7.2	1.0	0.0	2.4	8.0	3.9	6.9	-1.4
2-methyltetrahydrofuran	3.6	-0.6	8.5	4.6		1.9	12.5	7.7		2.6
tetrahydropyran	5.0	1.9	10.0	7.8	-3.5	1.6	10.8	9.5	10.9	6.2
1,3-dioxane		3.2		3.3		3.8		2.9	1.8	-0.5
1,3-dioxolan		4.9		5.6		2.4		5.3		3.2
1,8-cineole		2.8	19.3	19.4		0.5	19.7	22.3		18.9
anisole		11.0	15.7	18.4	1.9	2.4	17.4	17.0	19.1	16.1
ethyl phenyl ether		11.2	21.4	21.1	2.8	2.6	19.7	19.4	21.2	18.5
diphenyl ether		13.9	32.4	31.0		1.2	29.4	30.2		29.9
dibenzyl ether		11.0	31.1	37.8		1.0	24.3	37.3		36.9
1,2-dimethoxybenzene	5.8	9.2	17.3	22.3		1.7	14.5	21.5		20.6
methyl orthoformate		8.2		14.9		2.3	6.8	13.8		12.5
methyl orthoacetate		8.3		14.7		1.8		14.3		12.9
propionaldehyde	2.8	5.7	5.3	7.1	2.7	2.8	8.8	6.3	2.9	4.3
butyraldehyde	5.5	6.4	9.9	10.2	2.6	2.5	10.4	9.6	6.7	7.7
benzaldehyde		6.5	18.8	12.7	4.1	3.4	13.8	12.0	12.8	9.3
p-methoxybenzaldehyde		4.9		13.8		5.7	14.6	12.9		8.0
cinnamaldehyde		4.5	21.2	16.9		5.4	16.2	16.4		11.5
acetone		0.8	4.9	1.6	4.5	5.9	4.0	1.0	1.0	-4.3
2-butanone	2.9	1.5	6.5	5.4	3.1	4.1	7.0	5.8	4.4	1.3
2-pentanone	4.9	1.9	10.8	8.3	2.9	3.7	10.2	9.2	7.9	4.6
3-methyl-2-butanone	5.4	2.3	10.7	9.2		3.6	10.2	9.8	8.5	5.5
3-pentanone	5.4	2.1	12.2	9.0	2.4	3.2	10.1	9.9	8.7	5.8
cyclopentanone		0.8	6.8	7.1	7.1	4.0		8.0	5.1	3.2
4-methyl-2-pentanone	5.8	3.5	14.3	13.4		3.2	12.9	13.9		10.1
3,3-dimethyl-2-butanone	5.8	2.3	14.1	9.5	2.3	3.0	12.2	11.0	11.8	6.6
cyclohexanone	2.8	0.4	13.5	6.7	3.0	3.4	10.0	8.7	7.0	3.3
2-heptanone	6.2	3.1	18.1	19.3	2.6	3.4	16.7	19.9	15.6	15.9

3-heptanone	7.6	3.0	15.1	15.5		2.6		17.0		12.9
2,2,4,4-tetramethyl-3-pentanone		4.8		20.9		1.4	25.5	22.4		19.5
acetophenone	5.6	4.4	17.6	14.0	4.2	4.0	14.7	13.9	13.3	10.0
ethyl phenyl ketone	7.5	5.1	19.3	18.3		3.3	17.9	18.4		15.1
benzyl methyl ketone		4.7		15.7		4.2	13.6	15.7		11.5
2,4,5-trimethylacetophenone		3.3		16.2		3.6		16.9		12.6
p-chloroacetophenone		7.9		19.9		4.1	18.6	19.3		15.8
diphenyl ketone		4.3		22.4		3.6	23.5	23.2		18.8
2,4-pentanedione	3.9	4.9	8.3	5.4		7.9	7.3	2.0		-2.4
2,3-butanedione	3.9	6.8	6.1	7.2		6.8	-2.3	4.0		0.4
formic acid		3.3		3.8		11.2	2.3	5.8		-7.5
acetic acid		5.7	-1.5	6.4	10.6	11.1	4.4	7.0	-11.1	-4.8
propanoic acid		4.6	4.2	6.5	11.3	13.1	7.3	5.4	-7.1	-6.6
butanoic acid		5.3	8.3	9.4	11.8	12.4	9.9	8.7	-3.5	-2.9
pentanoic acid	1.9	6.0	13.5	12.8	12.3	11.7	13.3	12.6	0.4	1.1
hexanoic acid		6.5	16.1	16.0	13.5	11.3	16.3	16.2	3.2	4.7
heptanoic acid		7.0	20.1	19.3	14.1	10.9	19.2	19.7	6.6	8.4
dichloroacetic acid		1.5		8.4		13.8	10.6	15.2		-5.4
trifluoroacetic acid		-3.6		5.3		9.7		16.0		-4.4
acetic anhydride		6.3		8.0		6.7		5.8		1.3
benzoyl chloride		11.1		21.2		2.5		20.6		18.6
benzoyl bromide		11.7		20.4		2.0	22.1	20.4		18.4
methyl formate		4.9	6.2	5.1	3.1	4.5	5.6	3.1	3.6	0.6
ethyl formate	1.9	4.8	8.6	6.7	2.8	4.0	6.9	5.4	7.0	2.8
methyl acetate	3.3	3.2	6.5	5.0	2.9	4.0	6.4	4.2	4.9	1.0
ethyl acetate	5.1	3.2	10.0	7.1	2.6	4.0	9.6	6.7	8.2	3.1
n-propyl acetate	4.8	3.9	13.6	14.3	2.2	3.6	12.5	13.8	11.7	10.7
butyl acetate	6.5	4.4	17.0	17.6	2.1	3.4	15.5	17.2	15.1	14.2
i-pentyl acetate	6.7	4.6	20.3	17.2		3.0	23.5	17.6		14.2
methyl propionate		4.0	10.8	8.2	2.4	3.1	10.1	8.0	8.7	5.1
ethyl propionate	6.8	3.7	14.1	10.5	2.0	2.8	12.3	10.9	12.1	7.7
dimethyl carbonate	5.1	4.9	8.9	5.2		6.0		2.3		-0.8
diethyl carbonate	6.9	5.2	14.6	13.2		4.8	12.3	11.4		8.4
ethylene carbonate		3.0		2.7		13.4		-0.4		-10.8
4-methyl-1,3-dioxolan-2-one	2.7	3.0	8.2	4.2		11.8	3.0	1.7		-7.6
diethyl malonate		3.5	14.3	9.9		7.4	10.9	8.2		2.5
methyl benzoate	7.3	7.3	20.3	18.0	3.2	2.9	18.1	17.3	15.4	15.1
ethyl benzoate	8.0	7.1	24.1	20.6		2.7	20.5	20.2		17.9
dimethylphthalate		5.1	19.6	12.9		7.5	14.3	10.5		5.4
di-n-butylorthophthalate	6.7	5.9		35.4		5.1	32.3	34.7		30.3
ethyl chloroacetate	7.5	3.3	14.5	10.2		6.6	10.8	8.9		3.6
ethyl trichloroacetate		11.7		27.0		2.9	19.0	26.0		24.0
ethyl acetoacetate	3.2	4.9	9.9	14.0		6.8	6.8	11.7		7.2
γ-butyrolactone		-0.3		1.3		9.3	1.7	-0.4		-8.0
n-perfluorohexane	20.2	16.6	47.3	37.7		0.0		38.6		37.7
perfluoromethylcyclohexane		16.5		35.3		-0.5		37.0		35.8
perfluoroheptane	19.0	16.2	52.7	37.9		-0.6		40.4		38.5
perfluorooctane		16.6		44.7		-0.4		46.5		45.1
cis-perfluorodecalin		17.9		44.2		-1.2	39.6	45.2		45.5
fluorobenzene	15.8	16.4	20.2	19.5	0.3	0.0	18.3	19.6	19.8	19.5
hexafluorobenzene		17.0		26.3		0.2	19.9	26.2		26.1
1,4-dichlorobutane	13.6	14.8	21.0	22.3	0.1	1.2	18.2	21.4	18.7	21.1

chlorobenzene	15.4	16.0	23.4	24.0	0.4	0.5	21.6	23.6	22.9	23.5
dichloromethane	11.6	12.8	14.6	14.9	0.8	1.2	12.5	15.9	13.0	13.7
1,1-dichloroethane	13.0	13.8	17.2	15.3	0.5	1.0	15.6	15.7	16.8	14.2
1,2-dichloroethane	11.4	10.8	16.2	11.7	1.7	3.0	13.8	11.9	14.1	8.8
trans-1,2-dichloroethylene	14.5	14.8	16.7	17.3		0.5	17.3	18.3		16.9
o-dichlorobenzene	15.0	15.2	26.9	23.1	1.4	0.4	24.7	23.5	25.8	22.7
m-dichlorobenzene		16.0	27.8	27.6	0.5	0.6	25.5	27.6	27.2	27.0
chloroform	12.6	13.1	16.6	15.5		0.3	16.6	17.9	16.6	15.2
1,1,1-trichloroethane	14.8	15.7	21.4	21.1	5.6	0.5	19.6	21.4	21.8	20.6
1,1,2-trichloroethane	11.8	13.4	18.4	18.0	0.9	1.0	16.2	19.9	17.4	17.0
trichloroethylene	15.4	15.4	21.3	22.2		0.5	19.2	22.9		21.8
1,2,4-trichlorobenzene		15.8	30.5	27.3		0.2	28.3	28.2		27.1
carbon tetrachloride	16.8	16.3	23.1	20.7	-0.5	-0.2	21.5	21.8	23.3	20.9
tetrachloroethylene	17.2	16.8	24.5	23.2		-0.2	24.8	23.9		23.4
1,1,2,2-tetrachloroethane	11.4	13.1	20.0	19.4	1.2	0.8	20.6	22.9	18.7	18.6
pentachloroethane	13.8	13.9	24.8	22.5		0.3	23.8	25.5		22.2
1-bromobutane		15.1	23.4	21.5	0.4	0.8	21.1	21.0	23.0	20.6
bromobenzene	13.9	16.2	24.5	22.9	0.7	0.2	22.5	23.0	24.3	22.7
dibromomethane		13.3	16.7	16.4	1.7	1.2	16.1	17.4	15.0	15.2
1,2-dibromoethane	12.2	14.7	19.3	20.4	2.9	1.0	16.6	20.8	16.5	19.4
bromoform		13.2	20.8	17.6	1.4	0.7	16.6	20.3	19.5	16.9
n-butyl iodide			28.1		0.2		23.0		26.6	
iodobenzene	14.3		25.8		1.3		23.9		25.8	
methylene iodide	14.6		23.3		4.9		18.5		18.5	
n-butylamine		-2.5	4.5	14.1	1.2	4.8	10.4	16.5	3.3	9.3
benzylamine		-0.7	18.7	12.1		4.6	11.6	14.8		7.6
ethylenediamine		-4.2	-12.6	-1.9		14.1	-6.3	-0.7		-16.0
diethylamine		-4.5	4.1	13.7	0.2	3.2	8.7	17.0	3.5	10.5
di-n-butylamine	2.8	-3.3	18.2	28.3		2.2	21.5	32.0		26.1
pyrrole		5.7	10.9	5.0		7.9	9.7	5.3		-2.8
pyrrolidine		-9.8	1.1	7.0		4.5	8.0	12.5		2.5
piperidine		-4.3	4.3	10.5		2.6	10.2	14.5		7.9
morpholine		-1.1	-1.3	3.6		6.3	0.5	4.5		-2.8
triethylamine	3.8	-1.6	11.3	20.2	-0.6	0.2	13.7	23.5	6.6	19.9
tri-(n-butyl)amine	10.9	0.0	30.8	46.3		0.6	31.6	48.7		45.8
aniline	3.9	7.0	12.4	10.1	5.6	7.1	10.5	10.5	6.7	3.0
o-chloroaniline	8.1	8.6	16.6	15.5		5.1	16.2	18.0		10.4
methylphenylamine		8.5		13.5		4.9	14.9	12.9		8.6
N,N-dimethylaniline	6.1	11.9	21.6	20.7	1.1	1.9	18.6	19.4	19.6	18.8
aminoethanol		1.4		1.5		17.7	-2.1	-2.1		-16.2
diethanolamine		1.8	0.6	1.5		27.6	-2.8	-4.6		-26.1
triethanolamine		2.5		-1.2		31.5	-0.3	-6.7		-32.7
pyridine		-1.5	5.6	7.6	2.7	2.7	9.1	10.0	4.4	4.9
2-methylpyridine		-1.0	8.9	14.9	1.8	2.5	11.7	16.9	7.2	12.4
3-methylpyridine		-2.6	9.9	13.9	2.3	2.9	12.2	16.5	7.5	11.0
4-methylpyridine		-2.9	9.3	13.0	2.6	3.5	12.3	15.5	6.8	9.5
2,4-dimethylpyridine		-2.6	11.3	17.0	1.6	2.7	14.4	19.8	9.7	14.2
2,6-dimethylpyridine		-0.5	7.4	18.6	1.1	2.1	15.0	20.6	9.7	16.5
2,4,6-trimethylpyridine	0.5	-1.9	13.4	21.4		1.9	16.1	24.2		19.4
2-bromopyridine		4.0		13.9		4.1	13.5	14.0		9.9
3-bromopyridine		5.5		16.4		2.7	14.5	16.6		13.6
2-cyanopyridine		4.7		9.7		8.1	7.7	7.7		1.6

pyrimidine		1.4		4.2		5.2	3.1	4.0		-1.0
quinoline		1.5	17.5	16.8		2.4	17.0	18.7		14.4
acetonitrile		4.8	8.5	4.9	7.3	5.9	3.4	3.5	-0.5	-1.0
propionitrile		5.2	8.2	7.5	6.2	4.4	6.3	6.6	2.6	3.1
n-butyronitrile	9.4	5.8	11.7	10.6	5.1	3.8	8.4	10.1	6.2	6.8
3-methylbutanenitrile		6.5		15.1		3.3	11.5	14.6		11.8
acrylonitrile	6.1	6.1	9.0	6.4		4.7	6.8	5.7		1.7
phenylacetonitrile		8.1		17.7		3.6	14.3	17.6		14.1
benzonitrile	7.4	7.4	19.7	14.4	5.6	3.3	14.3	14.3	12.6	11.1
nitromethane	6.7	6.6	8.3	5.4	7.7	6.6	3.5	4.7	0.9	-1.1
nitroethane	7.8	8.2	11.1	9.8	6.3	5.9	6.4	8.0	4.9	3.9
1-nitropropane	8.7	10.1	14.3	14.6	5.4	4.1	10.4	13.6	9.2	10.5
2-nitropropane	9.1	9.1	14.0	14.5	5.7	4.1	10.0	12.5	8.4	10.3
nitrobenzene	10.2	9.3	20.3	17.1	5.3	3.6	15.9	16.2	15.1	13.5
formamide		2.1		0.4	22.0	28.7	-3.2	-6.8		-28.2
N-methylformamide		-2.3		0.5		16.4	-0.2	-1.4		-16.0
N,N-dimethylformamide		-4.3		-2.3		7.6	-0.4	-0.1		-10.0
N,N-dimethylthioformamide		4.4		6.5		9.6		2.6		-3.2
N,N-diethylformamide		-4.6		6.6		6.1		11.1		0.4
N-methylacetamide		-2.6	16.4	4.6		17.9	-0.6	3.1		-13.3
N,N-dimethylacetamide		-4.5	3.6	0.5		6.9	1.0	4.0		-6.3
N,N-diethylacetamide		-6.0		5.1		5.7	7.3	11.9		-0.6
2-pyrrolidinone		-4.6		0.5		15.5	0.5	1.4		-15.0
N-methyl pyrrolidinone		-6.4		0.7		5.7	2.3	6.6		-5.0
N-methyl thiopyrrolidinone		3.7		6.4		7.4		4.3		-1.0
tetramethylurea		-5.7		6.0		5.6	6.5	11.8		0.4
tetraethylurea		-0.5		17.5		2.3		22.3		15.1
dimethylcyanamide		2.1		6.1		7.7	4.5	4.2		-1.6
carbon disulfide	18.4	19.0	18.9	17.2		-0.2	16.5	16.9		17.4
dimethyl sulfide	10.6	10.1	12.7	10.9	-0.7	1.8	11.4	10.0	13.2	9.1
diethyl sulfide		11.6	18.2	18.7	-0.4	1.0	16.5	18.1	18.5	17.8
diisopropyl sulfide		12.4		26.9	-0.5	0.8	21.6	26.0	25.1	26.1
dibutyl sulfide		12.8		36.5		0.9		35.1		35.6
tetrahydrothiophene		10.5		17.2		1.6		16.1		15.6
thiane		11.6		18.3		0.9		17.8		17.4
dimethylsulfoxide		-5.6		-3.7		12.4	-2.3	-1.0		-16.1
dibutyl sulfoxide		-7.1		17.6		5.8		25.8		11.8
sulfolane		-0.2		0.0		12.0	1.0	-1.3		-12.0
thiobis(2-ethanol)		4.3		6.8		20.1		4.7		-13.3
diethyl sulfite		9.5		19.7		2.8		18.5		16.9
dimethyl sulfate		6.1	13.7	9.3		7.9	5.6	5.6		1.3
diethyl sulfate		5.9		12.3		6.9	11.9	9.6		5.4
methanesulfonic acid		3.3		3.3		22.2	-8.2	1.9		-18.9
trimethylphosphate		-3.7	-1.8	1.1		8.0	0.9	3.7		-6.9
triethylphosphate		-5.6	4.2	6.3		6.0	10.0	13.2		0.4
tri-n-butylphosphate	2.2	-9.0	26.2	23.2		4.7	28.2	35.9		18.5
hexamethylphosphoric triamide		-16.0		0.9		4.7	7.0	17.5		-3.7
hydrogen peroxide		0.9	-3.3	-0.8		22.0		-3.5		-22.8
hydrogen fluoride		-8.7		-4.1		11.6		3.6		-15.8
sulfuric acid		-6.7		-4.2		23.6		13.3		-27.9
ammonia		-8.2	-10.5	-4.7		10.8		-2.6	-7.1	-15.5
hydrazine		-3.4	1.5	-4.4		14.8		-7.3		-19.1

sulfur dioxide	7.5	5.5	3.3	7.6	2.1
thionyl chloride	8.3	7.4	1.6	15.3	5.8
phosphorus oxychloride	8.8	11.2	4.7	11.8	6.5