

Solvation thermodynamics data (Gibbs free energy, Enthalpy, Entropy) at 25 °C. Standard state of 1 mol/L for both gas and solution phases.

Data from:

Zanith, C. C.; Pliego, J. R., Jr., Performance of the SMD and SM8 models for predicting solvation free energy of neutral solutes in methanol, dimethyl sulfoxide and acetonitrile. *J Comput Aided Mol Des* **2015**, 29, 217-224.

<http://dx.doi.org/10.1007/s10822-014-9814-3>

Methanol solvent

Compound	exper		
	ΔH (kcal/mol)	ΔS (cal/K.mol)	ΔG(kcal/mol)
propane	-3.1	-6.8	-1.12
Propene	-3.4	-7.0	-1.29
Butane	-3.8	-6.9	-1.72
isobutane	-3.7	-7.2	-1.53
1-butene	-4.2	-7.8	-1.87
isobutene	-4.2	-7.8	-1.88
trans-2-butene	-4.2	-7.4	-1.97
cis-2-butene	-4.4	-7.7	-2.06
1,3-butadiene	-4.4	-7.5	-2.15
dimethylether	-4.0	-5.7	-2.31
chloroethane	-5.1	-8.3	-2.63
1,1-difluorethane	-4.0	-7.0	-1.90
Dichlorodifluoromethane	-3.8	-7.7	-1.49
Chlordifluoromethane	-4.7	-8.6	-2.12

Difluoromethane	-2.3	-2.6	-1.49
Chloropentafluoroethane	-2.6	-6.5	-0.60
Pentafluoroethane	-3.5	-6.4	-1.59
1.1.1.2- Tetrafluoroethane	-4.4	-8.3	-1.91
ethanol			-4.41
n-propanol			-4.75
i-propanol			-4.53
butanol			-5.31
benzene			-3.84
toluene			-4.38
ethylbenzene			-4.89
o-xylene			-4.92
m-xylene			-4.76
p-xylene			-4.76
n-pentane			-1.91
n-hexane			-2.47
n-heptane			-2.93
o-cresol			-7.72
m-cresol			-7.68
p-cresol			-7.84
o-toluidine			-7.54
m-toluidine			-7.75
γ-picoline			-5.60

Dimethyl sulfoxide solvent

Compound		exper	
	DH (kcal/mol)	DS (cal/K.mol)	DG(kcal/mol)
hexane	-4.1	-7.3	-1.87
heptane	-4.9	-8.5	-2.37
octane	-6.0	-10.4	-2.86
1-pentene	-4.2	-8.4	-1.65
1-hexene	-4.1	-6.4	-2.22
1-octene	-6.5	-11.3	-3.14
methanol	-9.2	-13.8	-5.08
ethanol	-8.8	-12.2	-5.18
1-propanol	-9.7	-13.5	-5.68
2-propanol	-9.4	-14.3	-5.14
diethyl ether	-5.0	-9.0	-2.33
diisopropyl ether	-5.6	-10.4	-2.49
tetrahydrofuran	-6.3	-8.9	-3.64
acetone	-6.7	-9.8	-3.76
2-butanone	-7.3	-10.6	-4.15
2-pentanone	-7.7	-10.9	-4.50
acetaldehyde	-5.6	-8.5	-3.04
vinyl acetate	-6.7	-9.5	-3.91
dichloromethane	-7.5	-11.5	-4.10
chloroform	-8.4	-12.3	-4.75
benzene	-6.9	-9.8	-3.96

Acetonitrile solvent

Compound		exper	
	DH (kcal/mol)	DS (cal/K.mol)	DG(kcal/mol)
ethanol			-4.32
n-propanol			-4.65
i-propanol			-4.39
butanol			-5.20
benzene			-4.25
toluene			-4.83
ethylbenzene			-5.36
o-xylene			-5.43
m-xylene			-5.28
p-xylene			-5.27
n-pentane			-2.08
n-hexane			-2.64
n-heptane			-3.10
o-cresol			-7.92
m-cresol			-7.90
p-cresol			-8.08
o-toluidine			-7.85
m-toluidine			-8.04
γ -picoline			-5.75

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