Minnesota Solvent Descriptor Database

Paul Winget, Derek M. Dolney, David J. Giesen, Christopher J. Cramer,
and Donald G. Truhlar
Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455-0431

version date: July 9, 1999; updated: June 6, 2010

This database contains tables of the solvent descriptors (defined below) that are used in the SM5 suite of universal solvation models[1–14] (SM5.0, SM5.2R, SM5.4, SM5.42R, SM5.42, and SM5CR) and in Vertical Excitation Model 42[15] (VEM42). The SM5.4 universal solvation model[1,2] requires n, α, β, γ, and ε, except for water[3] and chloroform[4] for which it only requires ε. The SM5.0R model[5,6] requires n, α, β, γ, ϕ, and ψ, except for water, for which no solvent descriptors are required. The SM5.2R,[7] SM5.42R,[8–11] SM5.42,[12,13] and SM5CR[14] models require requires n, α, β, γ, ε, ϕ, and ψ, except for water, which requires only ε. The VEM42 model[16] requires n_{25} and ε.

The descriptors are defined as follows

n index of refraction at optical frequencies at 293 K. This is sometimes called n_{20}^{D}.

α Abraham's hydrogen bond acidity. In particular, in Abraham's notation this is called $\Sigma\alpha_2^H$.

β Abraham's hydrogen bond basicity. In particular in Abraham's notation this is called $\Sigma\beta_2^H$.

γ $\gamma = \gamma_m/\gamma^o$, where γ_m is macroscopic surface tension at a liquid-air interface at 298 K, and γ^o is 1 cal mol^{-1} Å^{-2}. Conversion factor: 1 dyne/cm = 1.43932 cal mol^{-1} Å^{-2}.

ε dielectric constant at 298 K. Note that dielectric constant is also called relative permittivity.

ϕ aromaticity: fraction of non-hydrogenic solvent atoms that are aromatic carbon atoms.

ψ electronegative halogenicity: fraction of non-hydrogenic solvent atoms that are F, Cl, or Br.

n_{25} index of refraction at optical frequencies at 298 K. This is sometimes called n_{25}^{D}.

Some comments on possible points of confusion may be helpful. (1) Although the SM5 solvation models are parameterized for free energies of solvation at 298 K, the solvent descriptor *n* was chosen as n_{20}^{D} (which corresponds to 293 K) because it is more readily available. (2) The VEM42 model should use the correct index of refraction and dielectric constant at the temperature of the experiment under consideration, e.g., 298 K. (3) Technically (originally), the acidity and basicity descriptors used here are *solute* descriptors, but we use them as *solvent* descriptors.

The solvent descriptors *n*, α, β, γ, ε, φ, and ψ used for parameterization of the SM*x* universal solvation models are published in an original paper[2] and supporting information[14] for one of the original papers. In some cases we have subsequently updated the database to a more accurate value. We especially note that many of the dielectric constants have been updated to their correct values at 298 K.

The table that follows includes all solvents used to parameterize the SM*x* universal solvation models,[1–14] all liquids included in our article about the use of SM*x* models to predict vapor pressures,[16] and also many additional solvents.

If the goal is to reproduce calculations in the original papers[1–14] in order to test a program, the user should use the originally published values of the solvent descriptors. For all other purposes, including the use of SM*x* models for future applications, we recommend using the values in this database.

1 "A Universal Organic Solvation Model," D. J. Giesen, M. Z. Gu, C. J. Cramer, and D. G. Truhlar, Journal of Organic Chemistry **61**, 8720-8721 (1996).

2 "A Universal Solvation Model for the Quantum Mechanical Calculation of Free Energies of Solvation in Non-Aqueous Solvents," D. J. Giesen, G. D. Hawkins, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, Theoretical Chemistry Accounts **98**, 85-109 (1997); erratum: **101**, 309 (1999).

3 "Model for Aqueous Solvation Based on Class IV Atomic Charges and First-Solvation Shell Effects," C. C. Chambers, G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, Journal of Physical Chemistry **100**, 16385-16398 (1996).

4 "A Solvation Model for Chloroform Based on Class IV Atomic Charges," D. J. Giesen, C. C. Chambers, C. J. Cramer, and D. G. Truhlar, Journal of Physical Chemistry B **101**, 2061-2069 (1997).

5 "Parameterized Model for Aqueous Free Energies of Solvation Using Geometry-Dependent Atomic Surface Tensions with Implicit Electrostatics," G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, Journal of Physical Chemistry B **101**, 7147-7157 (1997).

6 "OMNISOL: Fast Prediction of Free Energies of Solvation and Partition Coefficients," G. D. Hawkins, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, Journal of Organic Chemistry **63**, 4305-4313 (1998).

[7] "Universal Quantum Mechanical Model for Solvation Free Energies Based on Gas-Phase Geometries," G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, Journal of Physical Chemistry B **102**, 3257-3271 (1998).

[8] "Density Functional Solvation Model Based on CM2 Atomic Charges," T. Zhu, J. Li, G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, Journal of Chemical Physics **109**, 9117-9133 (1998).

[9] "Universal Reaction Field Model Based on Ab Initio Hartree-Fock Theory," J. Li, G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, Chemical Physics Letters **288**, 293-298 (1998).

[10] "Extension of the Platform of Applicability of the SM5.42R Universal Solvation Model," J. Li, T. Zhu, G. D. Hawkins, P. Winget, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, Theoretical Chemistry Accounts, in press.

[11] "A Universal Solvation Model Based on Class IV Charges and the Intermediate Neglect of Differential Overlap for Spectroscopy Molecular Orbital Method," J. Li, T. Zhu, C. J. Cramer, and D. G. Truhlar, Journal of Physical Chemistry, submitted (for publication in W. A. Goddard III Birthday Issue).

[12] "Analytical Energy Gradients of a Self-Consistent Reaction-Field Solvation Model Based on CM2 Charges," T. Zhu, J. Li, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, Journal of Chemical Physics **110**, 5503-5513 (1999).

[13] "Direct Dynamics for Free Radical Kinetics in Solution: Solvent Effect on the Rate Constant for the Reaction of Methanol with Atomic Hydrogen," Y.-Y. Chuang, M. L. Radhakrishnan, P. L. Fast, C. J. Cramer, and D. G. Truhlar, Journal of Physical Chemistry **103**, 4893-4909 (1999).

[14] "A Universal Solvation Model Based on the Conductor-like Screening Model," D. M. Dolney, G. D. Hawkins, P. Winget, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, Journal of Computational Chemistry, submitted.

[15] "A Two-Response-Time Model Based on CM2/INDO/S2 Electrostatic Potentials for the dielectric Polarization Component of Solvatochromic Shifts on Vertical Excitation Energies," J. Li, C. J. Cramer, and D. G. Truhlar, International Journal of Quantum Chemistry, submitted (for the Festschrift in Honor of Michael C. Zerner's 60th birthday).

[16] "Prediction of Vapor Pressures from Self-Solvation Free Energies Calculated by the SM5 Series of Universal Solvation Models," P. Winget, G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, Journal of Physical Chemistry B, submitted.

Solvent	n	n_{25}	α, β	γ	ε	ϕ	ψ
1,1,1-trichloroethane	1.4379 [a]	1.4313 [b]	0.00, 0.09 [c]	36.24 [a]	7.0826 [a,d]	0.000	0.600
1,1,2-trichloroethane	1.4714 [a]	1.4689 [b]	0.13, 0.13 [c]	48.97 [a]	7.1937 [a]	0.000	0.600
1,2,4-trimethylbenzene	1.5048 [a]	1.5024 [b]	0.00, 0.19 [e]	42.03 [a]	2.3653 [a,d]	0.667	0.000
1,2-dibromoethane	1.5387 [a]	1.5364 [f]	0.10, 0.17 [c]	56.93 [a]	4.9313 [a,d]	0.000	0.500
1,2-dichloroethane	1.4448 [a]	1.4425 [f,g]	0.10, 0.11 [e]	45.86 [a]	10.125 [a,d]	0.000	0.500
1,2-ethanediol	1.4318 [a]	1.4306 [h]	0.58, 0.78 [i]	69.07 [a]	40.245 [a,d]	0.000	0.000
1,4-dioxane	1.4224 [a]	1.4204 [f,g]	0.00, 0.64 [c]	47.14 [a]	2.2099 [a,d]	0.000	0.000
1-bromo-2-methylpropane	1.4348 [a]	1.4349 [f]	0.00, 0.12 [e]	34.69 [f]	7.7792 [a,d]	0.000	0.200
1-bromooctane	1.4524 [a]	1.4500 [f]	0.00, 0.12 [e]	41.28 [j,k]	5.0244 [a,d]	0.000	0.111
1-bromopentane	1.4447 [a]	1.4420 [l]	0.00, 0.12 [e]	38.7 [j,k]	6.269 [a,d]	0.000	0.167
1-bromopropane	1.4343 [a]	1.4315 [f]	0.00, 0.12 [e]	36.36 [a]	8.0496 [a,d]	0.000	0.250
1-butanol	1.3993 [a]	1.3971 [b]	0.37, 0.48 [c]	35.88 [a]	17.332 [a,d]	0.000	0.000
1-chlorohexane	1.4199 [a]		0.00, 0.10 [e]	37.03 [a]	5.9491 [a,d]	0.000	0.143
1-chloropentane	1.4127 [a]	1.4104 [b]	0.00, 0.10 [e]	35.12 [a]	6.5022 [a,d]	0.000	0.167
1-chloropropane	1.3879 [a]	1.3851 [f,g]	0.00, 0.10 [c]	30.66 [a]	8.3548 [a,d]	0.000	0.250
1-decanol	1.4372 [a]	1.4353 [f]	0.37, 0.48 [m]	41.04 [a]	7.5305 [a,d]	0.000	0.000
1-fluorooctane	1.3935 [a]	1.3927 [f]	0.00, 0.10 [m]	33.92 [j,k]	3.89 [a,n]	0.000	0.111
1-heptanol	1.4249 [a]	1.4224 [h]	0.37, 0.48 [c]	38.5 [f]	11.321 [a,d]	0.000	0.000
1-hexanol	1.4178 [a]	1.4162 [h]	0.37, 0.48 [c]	37.15 [a]	12.51 [a,d]	0.000	0.000
1-hexene	1.3837 [a]	1.385 [b]	0.00, 0.07 [e]	25.76 [a]	2.0717 [a,d]	0.000	0.000
1-hexyne	1.3989 [a]	1.3957 [b]	0.12, 0.10 [c]	28.79 [a,g]	2.615 [a,d]	0.000	0.000
1-iodobutane	1.5001 [a]	1.4958 [o]	0.00, 0.15 [e]	40.65 [a]	6.173 [a,d]	0.000	0.000
1-iodohexadecane	1.4806 [a]		0.00, 0.15 [p]	46.48 [j,k]	3.5338 [a,d]	0.000	0.000
1-iodopentane	1.4959 [a]		0.00, 0.15 [e]	41.56 [j,k]	5.6973 [a,d]	0.000	0.000
1-iodopropane	1.5058 [a]	1.5027 [f,g]	0.00, 0.15 [c]	41.45 [j,k]	6.9626 [a,d]	0.000	0.000
1-nitropropane	1.4018 [a]	1.3996 [f]	0.00, 0.31 [c]	43.32 [j,k]	23.73 [a,d]	0.000	0.000
1-nonanol	1.4333 [a]	1.4319 [b]	0.37, 0.48 [m]	40.14 [a]	8.5991 [a,d]	0.000	0.000
1-octanol	1.4295 [a]	1.4279 [b]	0.37, 0.48 [c]	39.01 [a]	9.8629 [a,d]	0.000	0.000
1-pentanol	1.4101 [a]	1.4080 [b]	0.37, 0.48 [c]	36.5 [a]	15.13 [a]	0.000	0.000

Solvent	n	n_{25}	α, β	γ	ε	ϕ	ψ
1-pentene	1.3715 [a]	1.3684 [b]	0.00, 0.07 [e]	22.24 [a]	1.9905 [a,d]	0.000	0.000
1-propanol	1.3850 [a]	1.3837 [b]	0.37, 0.48 [c]	33.57 [a]	20.524 [a,d]	0.000	0.000
2,2,2-trifluoroethanol	1.2907 [a,q]		0.57, 0.25 [e]	42.02 [j,k]	26.726 [a,d]	0.000	0.500
2,2,4-trimethylpentane	1.3915 [a]	1.3889 [f]	0.00, 0.00 [e]	26.38 [b]	1.9358 [a,d]	0.000	0.000
2,4-dimethylpentane	1.3815 [a]	1.3788 [b]	0.00, 0.00 [e]	25.42 [b]	1.8939 [a,d]	0.000	0.000
2,4-dimethylpyridine	1.5010 [a]	1.4985 [f,g]	0.00, 0.63 [e]	46.86 [j,k]	9.4176 [a,d]	0.625	0.000
2,6-dimethylpyridine	1.4953 [a]	1.4952 [f]	0.00, 0.63 [e]	44.64 [j,k]	7.1735 [a,d]	0.625	0.000
2-bromopropane	1.4251 [a]	1.4219 [f,g]	0.00, 0.14 [c]	33.46 [a]	9.3610 [a,d]	0.000	0.250
2-butanol	1.3978 [a]	1.3949 [b]	0.33, 0.56 [e]	32.44 [a]	15.944 [a,d]	0.000	0.000
2-chlorobutane	1.3971 [a]	1.3941 [b]	0.00, 0.12 [c]	31.1 [j,k]	8.3930 [a,d]	0.000	0.200
2-heptanone	1.4088 [a]	1.4073 [h]	0.00, 0.51 [c]	37.6 [a]	11.658 [a,d]	0.000	0.000
2-hexanone	1.4007 [a]	1.3987 [b]	0.00, 0.51 [c]	36.63 [a]	14.136 [a,d]	0.000	0.000
2-methoxyethanol	1.4024 [a]	1.4003 [f]	0.30, 0.84 [c]	44.39 [a]	17.2 [a]	0.000	0.000
2-methyl-1-propanol	1.3955 [a]	1.3938 [b]	0.37, 0.48 [c]	32.38 [f]	16.777 [a,d]	0.000	0.000
2-methyl-2-propanol	1.3878 [a]	1.3852 [b]	0.31, 0.60 [e]	28.73 [a]	12.47 [a]	0.000	0.000
2-methylpentane	1.3715 [a]	1.3687 [b]	0.00, 0.00 [e]	24.3 [a]	1.89 [n,r]	0.000	0.000
2-methylpyridine	1.4957 [a]	1.4984 [f]	0.00, 0.58 [e]	47.5 [a]	9.9533 [a,d]	0.714	0.000
2-nitropropane	1.3944 [a]	1.3923 [f]	0.00, 0.33 [c]	42.16 [a]	25.654 [a,d]	0.000	0.000
2-octanone	1.4151 [a]	1.4133 [b]	0.00, 0.51 [e]	37.29 [b]	9.4678 [a,d]	0.000	0.000
2-pentanone	1.3895 [a]	1.3885 [f]	0.00, 0.51 [c]	33.46 [a]	15.200 [a,d]	0.000	0.000
2-propanol	1.3776 [a]	1.3752 [b]	0.33, 0.56 [c]	30.13 [a]	19.264 [a,d]	0.000	0.000
2-propen-1-ol	1.4135 [a]		0.38, 0.48 [e]	36.39 [a]	19.011 [a,d]	0.000	0.000
E-2-pentene	1.3793 [a]	1.3761 [b]	0.00, 0.07 [e]	23.62 [j]	2.051 [t,n]	0.000	0.000
3-methylpyridine	1.5040 [a]	1.5043 [f]	0.00, 0.54 [e]	49.61 [j,k]	11.645 [a,d]	0.714	0.000
3-pentanone	1.3924 [a]	1.3905 [h]	0.00, 0.51 [e]	35.61 [a]	16.78 [a,d]	0.000	0.000
4-heptanone	1.4069 [a]	1.4045 [b]	0.00, 0.51 [e]	35.98 [a]	12.257 [a,d]	0.000	0.000
4-methyl-2-pentanone	1.3962 [a]	1.394 [f,g]	0.00, 0.51 [e]	33.83 [b]	12.887 [a,d]	0.000	0.000
4-methylpyridine	1.5037 [a]	1.503 [l]	0.00, 0.54 [e]	50.17 [j,k]	11.957 [a,d]	0.714	0.000
5-nonanone	1.4195 [a]		0.00, 0.51 [e]	37.83 [a]	10.6 [n,s]	0.000	0.000

Solvent	n	n_{25}	α, β	γ	ε	ϕ	ψ
acetic acid	1.3720 [a]	1.3698 [b]	0.61, 0.44 [c]	39.01 [a]	6.2528 [a,d]	0.000	0.000
acetone	1.3588 [a]	1.3559 [f,g]	0.04, 0.49 [c]	33.77 [a]	20.493 [a,d]	0.000	0.000
acetonitrile	1.3442 [a]	1.3416 [f,g]	0.07, 0.32 [c]	41.25 [a]	35.688 [a,d]	0.000	0.000
acetophenone	1.5372 [a]	1.5321 [l]	0.00, 0.48 [c]	56.19 [a]	17.44 [a]	0.667	0.000
aniline	1.5863 [a]	1.5834 [f,g]	0.26, 0.41 [e]	60.62 [a]	6.8882 [a,d]	0.857	0.000
anisole	1.5174 [a]	1.5143 [b]	0.00, 0.29 [c]	50.52 [a]	4.2247 [a,d]	0.750	0.000
benzaldehyde	1.5463 [a]	1.5433 [f,g]	0.00, 0.39 [e]	54.69 [a]	18.220 [a,d]	0.857	0.000
benzene	1.5011 [a]	1.4972 [f,g]	0.00, 0.14 [c]	40.62 [a]	2.2706 [a,d]	1.000	0.000
benzonitrile	1.5289 [a]	1.5257 [t,u]	0.00, 0.33 [c]	55.83 [a]	25.592 [a,d]	0.750	0.000
benzyl alcohol	1.5396 [a]	1.5384 [h]	0.33, 0.56 [e]	52.96 [b]	12.457 [a,d]	0.750	0.000
bromobenzene	1.5597 [a]	1.5576 [f,g]	0.00, 0.09 [c]	50.72 [a]	5.3954 [a,d]	0.857	0.143
bromoethane	1.4239 [a]	1.4187 [f,g]	0.00, 0.12 [c]	34 [a]	9.01 [a]	0.000	0.333
bromoform	1.6005 [a]	1.5956 [b]	0.15, 0.06 [c]	64.58 [a]	4.2488 [a,d]	0.000	0.750
butanal	1.3843 [a]	1.3766 [b]	0.00, 0.45 [e]	35.06 [j,k]	13.45 [a]	0.000	0.000
butanoic acid	1.3980 [a]	1.3958 [b]	0.60, 0.45 [c]	37.49 [a]	2.9931 [a,d]	0.000	0.000
butanone	1.3788 [a]	1.3764 [b]	0.00, 0.51 [c]	34.5 [a]	18.246 [a,d]	0.000	0.000
butanonitrile	1.3842 [a]	1.382 [b]	0.00, 0.36 [e]	38.75 [a]	24.291 [a,d]	0.000	0.000
butyl ethanoate	1.3941 [a]	1.3923 [f]	0.00, 0.45 [c]	35.81 [a]	4.9941 [a,d]	0.000	0.000
butylamine	1.4031 [a]	1.3987 [b]	0.16, 0.61 [c]	33.74 [a]	4.6178 [a,d]	0.000	0.000
n-butylbenzene	1.4898 [a]	1.4874 [b]	0.00, 0.15 [e]	41.33 [j,k]	2.36 [r,g]	0.600	0.000
sec-butylbenzene	1.4895 [a]	1.4878 [b]	0.00, 0.16 [a b]	40.35 [j,k]	2.3446 [a,d]	0.600	0.000
tert-butylbenzene	1.4927 [a]	1.4902 [b]	0.00, 0.16 [e]	39.78 [j,k]	2.3447 [a,d]	0.600	0.000
carbon disulfide	1.6319 [a]	1.6241 [b]	0.00, 0.07 [e]	45.45 [a]	2.6105 [a,d]	0.000	0.000
carbon tetrachloride	1.4601 [a]	1.4574 [f]	0.00, 0.00 [e]	38.04 [a]	2.2280 [a,d]	0.000	0.800
chlorobenzene	1.5241 [a]	1.5221 [f,g]	0.00, 0.07 [c]	47.48 [a]	5.6968 [a,d]	0.857	0.143
chloroform	1.4459 [a]	1.4431 [b]	0.15, 0.02 [e]	38.39 [a]	4.7113 [a,d]	0.000	0.750
α-chlorotoluene	1.5391 [a]		0.00, 0.33 [c]	53.04 [j,k]	6.7175 [a,d]	0.750	0.125
o-chlorotoluene	1.5268 [a]	1.5233 [b]	0.00, 0.07 [c]	47.43 [b]	4.6331 [a,d]	0.750	0.125
m-cresol	1.5438 [a]	1.5394 [f]	0.57, 0.34 [c]	51.37 [a]	12.44 [a]	0.750	0.000

Solvent	n	n_{25}	α, β	γ	ε	ϕ	ψ
o-cresol	1.5361 [a]	1.5399 [f]	0.52, 0.30 [e]	53.11 [a]	6.76 [a]	0.750	0.000
cyclohexane	1.4266 [a]	1.4235 [b]	0.00, 0.00 [e]	35.48 [a]	2.0165 [a,d]	0.000	0.000
cyclohexanone	1.4507 [a]	1.4507 [b]	0.00, 0.56 [e]	49.76 [a]	15.619 [a,d]	0.000	0.000
cyclopentane	1.4065 [a]	1.4036 [b]	0.00, 0.00 [e]	31.49 [a]	1.9608 [a,d]	0.000	0.000
cyclopentanol	1.4530 [a]		0.32, 0.56 [e]	46.8 [j,k]	16.989 [a,d]	0.000	0.000
cyclopentanone	1.4366 [a]	1.4347 [f]	0.00, 0.52 [c]	47.21 [a]	13.58 [a]	0.000	0.000
decalin (*cis/trans* mixture)	1.4753 [a,w]	1.472 [f,h,w]	0.00, 0.00 [m,w]	43.82 [j,w]	2.196 [a,w]	0.000	0.000
cis-decalin	1.4810 [a]	1.4788 [f]	0.00, 0.00 [m]	45.45 [j,v]	2.2139 [a,d]	0.000	0.000
n-decane	1.4102 [a]	1.4094 [f]	0.00, 0.00 [e]	33.64 [a]	1.9846 [a,d]	0.000	0.000
dibromomethane	1.5420 [a]	1.5389 [b]	0.10, 0.10 [c]	56.21 [a]	7.2273 [a,d]	0.000	0.667
dibutylether	1.3992 [a]	1.3968 [f,g]	0.00, 0.45 [c]	35.98 [j]	3.0473 [a,d]	0.000	0.000
o-dichlorobenzene	1.5515 [a]	1.5491 [h]	0.00, 0.04 [c]	52.72 [b]	9.9949 [a,d]	0.750	0.250
E-1,2-dichloroethene	1.4454 [a]	1.4435 [f]	0.09, 0.05 [c]	37.13 [f]	2.14 [z]	0.000	0.500
Z-1,2-dichloroethene	1.4490 [a]	1.4461 [f,g]	0.11, 0.05 [c]	39.8 [f]	9.2 [r]	0.000	0.500
dichloromethane	1.4242 [a]	1.4212 [b]	0.10, 0.05 [e]	39.15 [a]	8.93 [a]	0.000	0.667
diethyl ether	1.3526 [a]	1.3496 [f]	0.00, 0.41 [c]	23.96 [a]	4.2400 [a,d]	0.000	0.000
diethyl sulfide	1.4430 [a]	1.4401 [f,g]	0.00, 0.32 [c]	35.36 [a]	5.723 [a]	0.000	0.000
diethylamine	1.3864 [a]	1.3825 [b]	0.08, 0.69 [c]	28.57 [a]	3.5766 [a,d]	0.000	0.000
diiodomethane	1.7425 [a]	1.738 [b]	0.05, 0.23 [c]	95.25 [j,k]	5.32 [a]	0.000	0.000
diisopropyl ether	1.3679 [a]	1.3653 [f,g]	0.00, 0.41 [e]	24.86 [a]	3.38 [x]	0.000	0.000
cis-1,2-dimethylcyclohexane	1.4360 [a]	1.4336 [b]	0.00, 0.00 [e]	36.28 [j,k]	2.06 [r]	0.000	0.000
dimethyl disulfide	1.5289 [a]	1.522 [f]	0.00, 0.28 [e]	48.06 [a]	9.6 [a]	0.000	0.000
N,*N*-dimethylacetamide	1.4380 [a]	1.4358 [h]	0.00, 0.78 [c]	47.62 [b]	37.781 [a,d]	0.000	0.000
N,*N*-dimethylformamide	1.4305 [a]	1.4280 [h]	0.00, 0.74 [c]	49.56 [t]	37.219 [a,d]	0.000	0.000
dimethylsulfoxide	1.4170 [a]	1.4773 [b]	0.00, 0.88 [e]	61.78 [a]	46.826 [a,d]	0.000	0.000
diphenylether	1.5787 [f]		0.00, 0.20 [c]	38.5 [a]	3.73 [a,y]	0.923	0.000
dipropylamine	1.4050 [a]	1.4018 [b]	0.08, 0.69 [c]	32.11 [a]	2.9112 [a,d]	0.000	0.000
n-dodecane	1.4216 [a]	1.4151 [b]	0.00, 0.00 [e]	35.85 [j,k]	2.0060 [a,d]	0.000	0.000
ethanethiol	1.4310 [a]	1.4278 [f]	0.00, 0.24 [m]	33.22 [a]	6.667 [a]	0.000	0.000

Solvent	n	n_{25}	α, β	γ	ε	ϕ	ψ
ethanol	1.3611 [a]	1.3593 [f]	0.37, 0.48 [c]	31.62 [a]	24.852 [a,d]	0.000	0.000
ethyl ethanoate	1.3723 [a]	1.3704 [b]	0.00, 0.45 [c]	33.67 [a]	5.9867 [a,d]	0.000	0.000
ethyl methanoate	1.3599 [f]	1.3575 [b]	0.00, 0.38 [c]	33.36 [a]	8.3310 [a,d]	0.000	0.000
ethyl phenyl ether	1.5076 [a]	1.5254 [f]	0.00, 0.32 [c]	46.65 [a]	4.1797 [a,d]	0.667	0.000
ethylbenzene	1.4959 [a]	1.4932 [h]	0.00, 0.15 [e]	41.38 [a]	2.4339 [a,d]	0.750	0.000
fluorobenzene	1.4684 [a]	1.4629 [b]	0.00, 0.10 [c]	38.37 [a]	5.42 [z]	0.857	0.143
formamide	1.4472 [a]	1.4468 [b]	0.62, 0.60 [c]	82.08 [a]	108.94 [a,d]	0.000	0.000
formic acid	1.3714 [a]	1.3693 [b]	0.75, 0.38 [c]	53.44 [a]	51.1 [a]	0.000	0.000
n-heptane	1.3878 [a]	1.3855 [h]	0.00, 0.00 [e]	28.28 [a]	1.9113 [a,d]	0.000	0.000
n-hexadecane	1.4345 [a]	1.4325 [b]	0.00, 0.00 [m]	38.93 [a]	2.0402 [a,d]	0.000	0.000
n-hexane	1.3749 [a]	1.3722 [f]	0.00, 0.00 [e]	25.75 [a]	1.8819 [a,d]	0.000	0.000
hexanoic acid	1.4163 [a]	1.4146 [f]	0.60, 0.45 [c]	39.65 [a]	2.6 [a]	0.000	0.000
iodobenzene	1.6200 [a]	1.6172 [f]	0.00, 0.12 [c]	55.72 [a]	4.5470 [a,d]	0.857	0.000
iodoethane	1.5133 [a]	1.5100 [f]	0.00, 0.15 [c]	40.96 [a]	7.6177 [a,d]	0.000	0.000
iodomethane	1.5380 [a]	1.5270 [b]	0.00, 0.13 [e]	43.67 [a]	6.8650 [a,d]	0.000	0.000
isopropylbenzene	1.4915 [a]	1.4889 [b]	0.00, 0.16 [e]	39.85 [b]	2.3712 [a,d]	0.667	0.000
p-isopropyltoluene	1.4909 [a]	1.4885 [b]	0.00, 0.19 [e]	38.34 [j,k]	2.2322 [a]	0.600	0.000
mesitylene	1.4994 [a]	1.4968 [b]	0.00, 0.19 [e]	39.65 [a]	2.2650 [a,d]	0.667	0.000
methanol	1.3288 [a]	1.3265 [b]	0.43, 0.47 [c]	31.77 [a]	32.613 [a,d]	0.000	0.000
methyl benzoate	1.5164 [a]	1.5146 [f]	0.00, 0.46 [c]	53.5 [a]	6.7367 [a,d]	0.600	0.000
methyl butanoate	1.3878 [a]	1.3847 [b]	0.00, 0.45 [c]	35.44 [a]	5.5607 [a,d]	0.000	0.000
methyl ethanoate	1.3614 [a]	1.3589 [b]	0.00, 0.45 [c]	35.59 [a]	6.8615 [a,d]	0.000	0.000
methyl methanoate	1.3433 [a]	1.3415 [b]	0.00, 0.38 [c]	35.06 [a]	8.8377 [a,d]	0.000	0.000
methyl propanoate	1.3775 [a]	1.3742 [f]	0.00, 0.45 [c]	35.18 [a]	6.0777 [a,d]	0.000	0.000
N-methylaniline	1.5684 [a]	1.5681 [f]	0.17,0.43 [e]	53.11 [a]	5.9600 [a,n]	0.750	0.000
methylcyclohexane	1.4231 [a]	1.4206 [b]	0.00, 0.00 [e]	33.52 [a]	2.024 [a,n]	0.000	0.000
N-methylformamide (*E/Z* mixture)	1.4319 [a]	1.4310 [f]	0.40, 0.55 [c]	55.44 [b]	181.56 [a,d]	0.000	0.000
nitrobenzene	1.5562 [a]	1.5030 [b]	0.00, 0.28 [c]	57.54 [r]	34.809 [a,d]	0.667	0.000
nitroethane	1.3917 [a]	1.3897 [f]	0.02, 0.33 [c]	46.25 [a]	28.29 [a,d]	0.000	0.000

Solvent	n	n_{25}	α, β	γ	ε	ϕ	ψ
nitromethane	1.3817 [a]	1.3796 [f,g]	0.06, 0.31 [c]	52.58 [a]	36.562 [a,d]	0.000	0.000
o-nitrotoluene	1.5450 [a]	1.5474 [b]	0.00, 0.27 [c]	59.12 [j,k]	25.669 [a,d]	0.600	0.000
n-nonane	1.4054 [a]	1.4031 [f]	0.00, 0.00 [e]	32.21 [a]	1.9605 [a,d]	0.000	0.000
n-octane	1.3974 [a]	1.3953 [f]	0.00, 0.00 [e]	30.43 [a]	1.9406 [a,d]	0.000	0.000
n-pentadecane	1.4315 [a]	1.4298 [b]	0.00, 0.00 [m]	38.34 [j,k]	2.0333 [a,d]	0.000	0.000
pentanal	1.3944 [a]	1.3917 [b]	0.00, 0.45 [c]	36.62 [a]	10.00 [a,n]	0.000	0.000
n-pentane	1.3575 [a]	1.3547 [b]	0.00, 0.00 [e]	22.3 [a]	1.8371 [a,n]	0.000	0.000
pentanoic acid	1.4085 [a]	1.4060 [b]	0.60, 0.45 [c]	38.4 [j,k]	2.6924 [a,d]	0.000	0.000
pentyl ethanoate	1.4023 [a]		0.00, 0.45 [c]	36.23 [a]	4.7297 [a,d]	0.000	0.000
pentylamine	1.448 [a]	1.4093 [b]	0.16, 0.61 [c]	35.54 [a]	4.2010 [a,d]	0.000	0.000
perfluorobenzene	1.3777 [a]	1.3761 [b]	0.00, 0.00	31.74 [b]	2.029 [a]	0.500	0.500
propanal	1.3636 [a]	1.3593 [b]	0.00, 0.45 [c]	32.48 [b]	18.5 [a,aa]	0.000	0.000
propanoic acid	1.3869 [a]	1.3848 [h]	0.60, 0.45 [c]	37.71 [a]	3.44 [a]	0.000	0.000
propanonitrile	1.3655 [a]	1.3633 [f]	0.02, 0.36 [c]	38.5 [a]	29.324 [a,d]	0.000	0.000
propyl ethanoate	1.3842 [a]	1.3822 [f]	0.00, 0.45 [c]	34.26 [a]	5.5205 [a,d]	0.000	0.000
propylamine	1.3870 [a]	1.3851 [b]	0.16, 0.61 [c]	31.31 [a]	4.9912 [a,d]	0.000	0.000
pyridine	1.5095 [a]	1.5073 [f,g]	0.00, 0.52 [e]	52.62 [a]	12.978 [a,d]	0.833	0.000
tetrachloroethene	1.5053 [a]	1.5055 [b]	0.00, 0.00 [c]	45.19 [f]	2.268 [a,ac]	0.000	0.667
tetrahydrofuran	1.4050 [a]	1.4044 [f,g]	0.00, 0.48 [c]	39.44 [f]	7.4257 [a,d]	0.000	0.000
tetrahydrothiophene-*S*,*S*-dioxide	1.4833 [a]		0.00, 0.88	87.49 [j,k]	43.962 [a,d]	0.000	0.000
tetralin	1.5413 [a]	1.5392 [h]	0.00, 0.19	47.74 [a]	2.771 [a]	0.600	0.000
thiophene	1.5289 [a]	1.5268 [h]	0.00, 0.15 [e]	44.16 [a]	2.7270 [a,d]	0.800	0.000
thiophenol	1.5893 [a]	1.5805 [f]	0.09, 0.16 [e]	55.24 [j,k]	4.2728 [a,d]	0.857	0.000
toluene	1.4961 [a]	1.4936 [f,g]	0.00, 0.14 [c]	40.2 [a]	2.3741 [a,d]	0.857	0.000
trans-decalin	1.4695 [a]	1.4671 [h]	0.00, 0.00 [m]	42.19 [j,v]	2.1781 [a,d]	0.000	0.000
tributylphosphate	1.4224 [a]	1.4215 [h]	0.00, 1.21 [e]	27.55 [r,n]	8.1781 [a,d]	0.000	0.000
trichloroethene	1.4773 [a]	1.4556 [f]	0.08, 0.03 [c]	41.45 [f]	3.422 [a,d]	0.000	0.600
triethylamine	1.4010 [a]	1.3980 [b]	0.00, 0.79 [e]	29.1 [a]	2.3832 [a,d]	0.000	0.000
n-undecane	1.4398 [a]	1.4151 [f]	0.00, 0.00 [e]	34.85 [a]	1.9910 [a,d]	0.000	0.000

Solvent	n	n_{25}	α, β	γ	ε	ϕ	ψ
water	1.3328 [a]	1.3323 [a,v]			78.355 [a,d]		
xylene (mixture)	1.4995 [a,ad]	1.4969 [b,ad]	0.00, 0.16 [m,ad]	41.38 [a,ad]	2.3879 [a,ad,d]	0.750	0.000
m-xylene	1.4972 [a]	1.4946 [b]	0.00, 0.16 [m]	40.98 [a]	2.3478 [a,d]	0.750	0.000
o-xylene	1.5055 [a]	1.5029 [b]	0.00, 0.16 [m]	42.83 [a]	2.5454 [a,d]	0.750	0.000
p-xylene	1.4958 [a]	1.4932 [b]	0.00, 0.16 [m]	40.32 [a]	2.2705 [a,d]	0.750	0.000

[a] *CRC Handbook of Chemistry and Physics*, 76th ed.; Weast, R. C., Ed.; CRC Press: Boca Raton, FL, 1995.

[b] Daubert,T. E.; Danner, R. P. *Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation*; Hemisphere Pub. Corp.: Bristol, PA, 1989.

[c] Abraham, M. H. *J. Phys. Org. Chem*. **1993**, *6*, 660-684.

[d] Computed from the equation $\varepsilon(T) = a + bT + cT^2 + dT^3$ where T is temperature in Kelvin.

[e] Abraham, M. H.; Chadha, H. S.; Whiting, G. S.; Mitchell, R. C. *J. Pharm. Sci*. *1994*, *83*, 1085-1100.

[f] *Beilstein: Handbook of Organic Chemistry*, 4th ed.; Luckenback, R., Ed. Springer-Verlag: New York 1984.

[g] Average of the values listed.

[h] *The Merck Index: an Encyclopedia of Chemicals, Drugs, and Biologicals*; 11th ed.; Budavari, S.; Ed.; Merck & Co.: Rahway, NJ, 1989.

[i] Abraham, M. H.; Rafols, C. *J. Chem. Soc., Perkin Trans. 2* **1995**, 1843-1851.

[j] Jasper, J. J. *J. Phys. Chem. Ref. Data* **1972**, *1*, 841.

[k] Computed from the equation $\gamma_m = a - bT$ where T is in ˚C.

[l] *Landolt-Börnstein: Numerical Data and Functional Relationships in Science and Technology*; 2nd ed.; D'ans, J., Eucken, A., Joos, G., Roth, W. A., Bartels, J., Borchers, H., Tenbruggencote, P., Hansen, H., Hellwege, K. H., Schäfer, K. L., Schmidt, E., Eds.; Springer-Verlag: Berlin, 1961.

[m] Abraham, M. H. *Chem. Soc. Rev*. **1993**, 73-83.

[n] Value at 20˚C.

[o] Artal, M.; Embid, J. M.; Velasco, I. *J. Chem. Thermodyn*. **1994**, *26*, 703-708.

[p] Taken to be the same as 1-iodoheptane. Abraham, M. H.; Chadha, H. S.; Whiting, G. S.; Mitchell, R. C. *J. Pharm. Sci*. **1994**, *83*, 1085-1100.

Solvent	n	n_{25}	α, β	γ	ε	ϕ	ψ

[q] Value at 22˚C.

[r] Lide, D. R. *Handbook of Organic Solvents*; CRC Press: Boca Raton, FL, 1995.

[s] *CRC Handbook of Chemistry and Physics*; 77 ed.; Weast, R. C., Ed.; CRC Press: Boca Raton, FL, 1996.

[t] *Organic Solvents: Physical Properties and Methods of Purification*, 3d ed.; Riddick, J., Bunger, W. B., Eds.; Wiley-Interscience: New York, 1970.

[u] Value at 25.5˚C.

[v] Listed data fit to quadratic function.

[w] Average of *cis* and *trans* decalin.

[x] *Handbook of Analytical Chemistry*, 1st ed.; Meites, L. Ed., McGraw-Hill: New York, 1963.

[y] Value at 10˚C.

[z] *American Institute of Physics Handbook*; 3rd ed.; Gray D.E. Ed.; McGraw-Hill: New York, 1972.

[aa] Value at 17˚C.

[ab] Abraham, M. H.; Andonian-Haftvan, J.; Whiting, G. S.; Leo, A.; Taft, R. S. *J. Chem. Soc., Perkin Trans. 2* **1994**, 1777-1791.

[ac] Value at 30˚C.

[ad] Average of *ortho*, *meta*, and *para* xylene.