

JOC 63 3821 worked out example	CHCl <sub>3</sub>	C <sub>6</sub> H <sub>6</sub>	2ME	DMF	DMSO	H <sub>2</sub> O	
density, g cm <sup>-3</sup>	1.490	1.492	0.876	0.965	0.944	1.100	1.000
[solvent], mol dm <sup>-3</sup>	12.5	12.5	11.2	12.7	12.9	14.1	55.5
numeral density rel. to ideal gas	2.806E-06	2.801E-06	2.514E-06	2.842E-06	2.895E-06	3.156E-06	1.244E-05
V <sup>free,macro</sup> 1 L occupies, cm <sup>3</sup>	7.5	7.5	6.8	7.6	7.8	8.5	33.4
V available for a solvent, Å <sup>3</sup>	132.6	132.9	148.1	131.0	128.6	117.9	29.9
Inter Solvent Distance, Å	5.10	5.10	5.29	5.08	5.05	4.90	3.10
V of a molecule, Å <sup>3</sup>	97	104	107	102	101	96	25
solvent radius, Å		2.920	2.945	2.895	2.889	2.840	1.814
MOPAC PM7 COSMO V, Å <sup>3</sup>		104	107	101	101	96	25
MOPAC PM7 COSMO A, Å <sup>2</sup>		116	119	117	115	110	42
G16PCM cavity V, Å <sup>3</sup>		141	134	111	125	111	19
G16PCM cavity A, Å <sup>2</sup>		145	143	124	138	124	36
SMD Rsolv, Å		2.48	2.63	2.46		2.46	1.39
SMD Vmol, Å <sup>3</sup>		80.70	88.91	70.94		70.94	18.07
R(solvent molecule), Å	4.59	4.71	4.75	4.67	4.66	4.58	2.92
V(non-excluded void), Å <sup>3</sup>	36	29	41	29	28	22	5
R(free), Å	1.01	0.73	1.09	0.82	0.72	0.60	0.33
V <sup>free.nano</sup> for single, Å <sup>3</sup>	1.03	0.39	1.28	0.56	0.37	0.22	0.04
shape: 8=cube; 6.3 sphere	8	6.3	8	8	6.3	6.3	6.3
M <sub>w</sub> (solvent), g mol <sup>-1</sup>	119.0	119.4	78.1	76.1	73.1	78.1	18.0
gas phase			36.9+12.5lnM+12.5lnT				
standard state, [X] mol dm <sup>-3</sup>	0.0446	0.0446	0.0446	0.0446	0.0446	0.0446	0.0446
approx. S <sub>trans</sub> , J mol <sup>-1</sup> K <sup>-1</sup>	167.9	168.0	162.7	162.3	161.8	162.7	144.3
part 1, Eq.2 in JOC 63 3821	-233.2	-233.2	-233.2	-233.2	-233.2	-233.2	-233.2
part 2, Eq.2 in JOC 63 3821	253.3	253.3	252.7	252.7	252.6	252.7	250.5
exact S <sub>trans</sub> , J mol <sup>-1</sup> K <sup>-1</sup>	167.6	167.7	162.4	162.0	161.5	162.4	144.1
exact S <sub>trans</sub> , cal mol <sup>-1</sup> K <sup>-1</sup>	40.1	40.1	38.8	38.8	38.6	38.8	34.5
solutions	solute trans. S, has to be dominated by SOLVENT molecules						
[analyte], 10 <sup>-3</sup> mol dm <sup>-3</sup>	1000	0.1	0.1	0.1	0.1	0.1	0.1
M <sub>w</sub> (analyte), g mol <sup>-1</sup>	32.0	33.0	33.0	33.0	33.0	33.0	33.0
[analyte] <sup>eff.</sup> , mol dm <sup>-3</sup>	132.620	0.013	0.015	0.013	0.013	0.012	0.003
simple model			11.1+12.5lnM+12.5lnT				
approx. S <sub>trans</sub> , J mol <sup>-1</sup> K <sup>-1</sup>	126	203	203	203	203	203	203
using [analyte] <sup>eff</sup> or V <sup>free</sup>		11.1+12.5lnM+12.5lnT-8.1ln[analyte, effective]					
approx. S <sub>trans</sub> , J mol <sup>-1</sup> K <sup>-1</sup>	85	162	161	162	162	163	174
change	68%	80%	79%	80%	80%	80%	86%
approx. S <sub>trans</sub> , J mol <sup>-1</sup> K <sup>-1</sup>	85.0	162.0	161.1	162.1	162.2	162.9	174.4
part 1, Eq.2 in JOC 63 3821	-241.2	-232.0	-232.1	-232.0	-231.9	-231.8	-230.5
part 2, Eq.2 in JOC 63 3821	251.4	251.4	251.4	251.4	251.4	251.4	251.4
exact S <sub>trans</sub> , J mol <sup>-1</sup> K <sup>-1</sup>	84.8	161.7	160.8	161.8	162.0	162.7	174.1
exact S <sub>trans</sub> , cal mol <sup>-1</sup> K <sup>-1</sup>	20.3	38.7	38.5	38.7	38.7	38.9	41.6
Free energy correction kJ mol <sup>-1</sup>	-12.1	-12.1	-12.4	-12.1	-12.0	-11.8	-8.4