

Avogadro's number, mol<sup>-1</sup> 6.02E+023  
 ideal gas constant, J mol<sup>-1</sup> K<sup>-1</sup> 8.315  
 Planck constant, Js 6.63E-034  
 temperature, K 298.15  
 ideal gas numeral density, m<sup>-3</sup> 2.69E+027

1 mol = 22.41 dm<sup>3</sup>

JOC 63 3821 worked out example ↓	CHCl <sub>3</sub>	CH <sub>2</sub> Cl <sub>2</sub>	C <sub>6</sub> H <sub>6</sub>	NEt <sub>3</sub>	MeOEtOH	DMF	acetone	THF	GBL	DMSO	CH <sub>3</sub> OH	H <sub>2</sub> O	[C <sub>2</sub> MIM] <sup>+</sup>	[NTf <sub>2</sub> ] <sup>-</sup>
density, g cm <sup>-3</sup>	1.490	1.492	1.325	0.876	0.726	0.965	0.944	0.791	0.889	1.130	1.100	0.791	1.000	1.524
[solvent], mol dm <sup>-3</sup>	12.5	12.5	15.6	11.2	7.2	12.7	12.9	13.6	12.3	13.1	14.1	24.7	55.5	3.9
numeral density rel. to ideal gas	2.806E-06	2.801E-06	3.497E-06	2.514E-06	1.607E-06	2.842E-06	2.895E-06	3.053E-06	2.763E-06	2.942E-06	3.156E-06	5.534E-06	1.244E-05	8.727E-07
V <sup>free,macro</sup> 1 L occupies, cm <sup>3</sup>	7.5	7.5	9.4	6.8	4.3	7.6	7.8	8.2	7.4	7.9	8.5	14.9	33.4	2.3
V available for a solvent, Å <sup>3</sup>	132.6	132.9	106.4	148.1	231.6	131.0	128.6	121.9	134.7	126.5	117.9	67.3	29.9	426.5
Inter Solvent Distance, Å	5.10	5.10	4.74	5.29	6.14	5.08	5.05	4.96	5.13	5.02	4.90	4.07	3.10	7.53
V of a molecule, Å <sup>3</sup>	97	104	82	107	161	102	101	85	98	103	96	47	25	401
solvent radius, Å	2.920	2.695	2.945	3.375	2.895	2.889	2.728	2.858	2.909	2.840	2.239	1.814	4.575	
MOPAC PM7 COSMO V, Å <sup>3</sup>	104	82	107	160	101	101	85	98	103	96	47	25	401	
MOPAC PM7 COSMO A, Å <sup>2</sup>	116	97	119	159	117	115	101	111	116	110	66	42	323	
G16PCM cavity V, Å <sup>3</sup>	141	108	134	196	111	125	89	99	122	111	39	19	346	
G16PCM cavity A, Å <sup>2</sup>	145	119	143	201	124	138	110	116	134	124	60	36	369	
SMD Rsolv, Å	2.48	2.27	2.63	2.39	2.46	n/a	2.38	2.56	2.44	2.46	1.86	1.39	4.82	
SMD Vmol, Å <sup>3</sup>	80.70	64.50	88.91	126.25	70.94	n/a	73.52	81.11	81.45	70.94	40.70	18.07	401.20	
R(solvent molecule), Å	2.85	2.92	2.70	2.95	3.37	2.89	2.89	2.73	2.86	2.91	2.84	2.24	1.81	4.57
V(non-excluded void), Å <sup>3</sup>	36	29	24	41	71	29	28	37	37	23	22	20	5	25
R(free), Å	4.50	4.03	3.78	4.33	5.11	4.03	3.99	4.12	4.19	3.90	3.81	3.38	2.38	5.45
V <sup>free,nano</sup> for single, Å <sup>3</sup>	91.04	65.50	53.80	81.27	133.37	65.60	63.34	69.97	73.52	59.28	55.36	38.49	13.54	162.16
shape: 8 for cube; 6.3 sphere	8	6.3	6.3	6.3	6.3	6.3	6.3	6.3	6.3	6.3	6.3	6.3	6.3	6.3
M <sub>w</sub> (solvent), g mol <sup>-1</sup>	119.0	119.4	84.9	78.1	101.2	76.1	73.1	58.1	72.1	86.1	78.1	32.0	18.0	391.3
gas phase	36.9 + 12.5 ln M + 12.5 ln T													
standard state, [X] mol dm <sup>-3</sup>	0.0446	0.0446	0.0446	0.0446	0.0446	0.0446	0.0446	0.0446	0.0446	0.0446	0.0446	0.0446	0.0446	0.0446
approx. S <sub>trans</sub> <sup>+</sup> J mol <sup>-1</sup> K <sup>-1</sup>	167.9	168.0	163.7	162.7	165.9	162.3	161.8	159.0	161.7	163.9	162.7	151.5	144.3	182.8
part 1, Eq.2 in JOC 63 3821	-233.2	-233.2	-233.2	-233.2	-233.2	-233.2	-233.2	-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	252.8	252.7	253.1	252.7	252.6	252.3	252.6	252.9	252.7	251.4	250.5	255.1
exact S <sub>trans</sub> <sup>+</sup> J mol <sup>-1</sup> K <sup>-1</sup>	167.6	167.7	163.4	162.4	165.6	162.0	161.5	158.7	161.4	163.6	162.4	151.3	144.1	182.5
exact S <sub>trans</sub> <sup>+</sup> cal mol <sup>-1</sup> K <sup>-1</sup>	40.1	40.1	39.1	38.8	39.6	38.8	38.6	38.0	38.6	39.1	38.8	36.2	34.5	43.7
liquid phase	-8.0 + 12.5 ln M + 12.5 ln T													
[X], mol dm <sup>-3</sup>	10	12.5	15.6	11.2	7.2	12.7	12.9	13.6	12.3	13.1	14.1	24.7	55.5	3.9
approx. S <sub>trans</sub> <sup>+</sup> J mol <sup>-1</sup> K <sup>-1</sup>	122.9	121.1	115.0	116.7	123.7	115.4	114.7	111.4	114.9	116.6	114.8	99.0	85.1	145.6
exact S <sub>trans</sub> <sup>+</sup> J mol <sup>-1</sup> K <sup>-1</sup>	-238.6	-238.8	-239.0	-238.7	-238.3	-238.8	-238.8	-238.9	-238.8	-238.9	-238.9	-239.5	-240.3	-237.6
exact S <sub>trans</sub> <sup>+</sup> cal mol <sup>-1</sup> K <sup>-1</sup>	253.3	253.3	252.8	252.7	253.1	252.7	252.6	252.3	252.6	252.9	252.7	251.4	250.5	255.1
exact S <sub>trans</sub> <sup>+</sup> J mol <sup>-1</sup> K <sup>-1</sup>	122.6	120.8	114.7	116.4	123.4	115.1	114.4	111.1	114.6	116.3	114.5	98.7	84.8	145.3
condensation entropy, J mol <sup>-1</sup> K <sup>-1</sup>	-45.0	-46.9	-48.7	-46.0	-42.2	-47.0	-47.1	-47.6	-46.7	-47.3	-47.8	-52.5	-59.3	-37.2
exp. estimate, J mol <sup>-1</sup> K <sup>-1</sup>							-88.0							
improved liquid phase	solvent effectively more concentrated w/respect to translational S; thus consider non-excluded vs. V <sup>free</sup>													
corrected [X] mol dm <sup>-3</sup>	15	25	31	20	12	25	26	24	23	28	30	43	123	10
approx. S <sub>trans</sub> <sup>+</sup> J mol <sup>-1</sup> K <sup>-1</sup>	122.9	121.1	115.0	116.7	123.7	115.4	114.7	111.4	114.9	116.6	114.8	99.0	85.1	145.6
part 1, Eq.2 in JOC 63 3821	-239.0	-239.5	-239.7	-239.3	-238.8	-239.5	-239.6	-239.5	-239.4	-239.6	-239.7	-240.1	-241.1	-238.6
part 2, Eq.2 in JOC 63 3821	253.3	253.3	252.8	252.7	253.1	252.7	252.6	252.3	252.6	252.9	252.7	251.4	250.5	255.1
exact S <sub>trans</sub> <sup>+</sup> J mol <sup>-1</sup> K <sup>-1</sup>	119.5	114.9	109.0	111.4	118.8	109.3	108.5	106.5	109.6	110.0	108.2	94.1	78.2	137.3
S of condensation, J mol <sup>-1</sup> K <sup>-1</sup>	-48.1	-52.7	-54.4	-50.9	-46.8	-52.7	-53.0	-52.2	-51.8	-53.6	-54.1	-57.2	-65.8	-45.2
exp. estimate, J mol <sup>-1</sup> K <sup>-1</sup>							-88.0							
solutions	solute translational 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	0.1	0.1	0.1	0.1	0.1	0.1	0.1
M <sub>w</sub> (analyte), g mol <sup>-1</sup>	32.0	32.0	32.0	32.0	32.0	32.0	32.0	32.0	32.0	32.0	32.0	32.0	32.0	32.0
[analyte] <sup>eff</sup> , mol dm <sup>-3</sup>	132.620	0.013	0.011	0.015	0.023	0.013	0.013	0.012	0.013	0.013	0.012	0.007	0.003	0.043
simplified model, using [analyte]	11.1 + 12.5 ln M + 12.5 ln T													
approx. S <sub>trans</sub> <sup>+</sup> J mol <sup>-1</sup> K <sup>-1</sup>	126	202	202	202	202	202	202	202	202	202	202	202	202	202
using [analyte] <sup>eff</sup> or V <sup>free</sup>	11.1 + 12.5 ln M + 12.5 ln T - 8.1 ln [analyte] <sup>effective</sup>													
approx. S <sub>trans</sub> <sup>+</sup> J mol <sup>-1</sup> K <sup>-1</sup>	85	162	163	161	157	162	162	162	161	162	163	167	174	152
change	68%	80%	81%	79%	78%	80%	80%	80%	80%	80%	80%	83%	86%	75%
approx. S <sub>trans</sub> <sup>+</sup> J mol <sup>-1</sup> K <sup>-1</sup>	85.0	161.6	163.4	160.7	156.9	161.7	161.8	162.3	161.5	162.0	162.6	167.2	174.0	151.9
part 1, Eq.2 in JOC 63 3821	-241.2	-232.0	-231.7	-232.1	-232.5	-232.0	-231.9	-231.9	-232.0	-231.9	-231.8	-231.3	-230.5	-233.1
part 2, Eq.2 in JOC 63 3821	251.4	251.4	251.4	251.4	251.4	251.4	251.4	251.4	251.4	251.4	251.4	251.4	251.4	251.4
exact S <sub>trans</sub> <sup>+</sup> J mol <sup>-1</sup> K <sup>-1</sup>	84.8	161.3	163.2	160.4	156.7	161.4	161.6	162.0	161.2	161.7	162.3	167.0	173.7	151.6
exact S <sub>trans</sub> <sup>+</sup> cal mol <sup>-1</sup> K <sup>-1</sup>	20.3	38.6	39.0	38.4	37.5	38.6	38.7	38.8	38.6	38.7	38.8	39.9	41.6	36.3
Free energy correction kJ mol <sup>-1</sup>	-12.1	-12.1	-11.6	-12.4	-13.5	-12.1	-12.0	-11.9	-12.2	-12.0	-11.8	-10.4	-8.4	-15.0