Title
Predicting cavity formation free energy: how far is the Gaussian approximation valid?

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iAMOEBA	260K	273K	285K	298K	310K	323K
Stat Time (ns)	10	10	10	10	5	5
Pressure (atm)	1.04	1.41	1.04	1.14	1.18	1.21
Binding Energy (kcal/mol)	-2349.02	-2299.96	-2252.95	-2205.10	-2160.84	-2121.26
Density (g/cc)	0.9995 (0.99714)	1.0032 (0.99981)	1.0036 (0.99953)	0.9995 (0.99716)	0.9938 (0.99362)	0.9876 (0.98838)
Hvap (kcal/mol)	11.234 (10.9029)	11.001 (10.7732)	10.779 (10.6483)	10.549 (10.5176)	10.336 (10.3986)	10.140 (10.2640)
κ_T(10-6 atm-1)	78.8	71.1 (51.62)	65.8	60.5 (45.86)	60.7	64.1 (44.76)
C_p (cal/mol/K)	20.8 (18.38)	19.8 (18.170)	19.3 (18.048)	18.6 (18.004)	18.5 (17.995)	18.3 (18.004)
αp (10-4 K-1)	-4.4 (-3.712)	-1.4 (-0.705)	2.1 (1.185)	3.7 (2.556)	5.0 (3.648)	6.0 (4.567)
Dielectric constant						

B90	250K	275K	300K	350K	400K	450K	500 K	550 K
Stat Time (ns)	0.82	0.84	0.86	0.90	0.98	1.08		
Pressure (atm)	1.3	2.7	1.5	-1.7	2.4	1.4		
Binding E(kcal/mol)	-14691.4	-14174.1	-13681.1	-12697.1	-11679.8	-10495.9		
Density (g/cc)	1.084	1.045	1.006	0.918	0.817	0.679		
Hvap	8.303	8.028	7.764	7.222	6.631	5.858		
K_T(10-6 atm-1)	59.44	74.47	89.91	143.0	259.3	806.6		
C_p (cal/mol/K)	12.12	11.31	11.24	11.55	12.29	16.16		
αp (10-4 K-1)	14.18	14.78	16.26	20.66	27.27	52.83		
Dielectric constant	1339.0	370.0	231.0	114.9	65.0	35.7		

B105	250K	275K	300K	350K	400K	450K	500K	550 K
Stat Time (ns)	0.82	0.82	0.83	0.86	0.89	0.93	1.00	
Pressure (atm)	1.4	0.20	0.24	2.36	3.2	-1.4	3.8	
Binding E(kcal/mol)	-17985.1	-17389.4	-16818.7	-15705.2	-14593.3	-13424.0	-12100.6	
Density (g/cc)	1.033	1.016	0.997	0.948	0.888	0.812	0.710	
Hvap	10.175	9.868	9.573	8.989	8.391	7.734	6.935	
K_T(10-6 atm-1)	48.49	51.73	53.29	72.22	98.35	175.6	416.5	
C_p (cal/mol/K)	13.63	13.50	12.92	12.59	12.99	14.00	17.55	
αp (10-4 K-1)	5.54	7.66	8.23	11.63	14.65	21.06	37.41	
Dielectric constant	134.0	112.5	88.13	70.6	51.7	39.8	26.6	