

	AA	PX	CapSH RX	TS	PX	CySH RX	TS	PX	GSH RX	TS
E _(g) / Hartree	-247.404390	-1278.380054	-1030.946135	-1278.288852	-969.567652	-722.134999	-969.479642	-1653.089804	-1405.663242	-1653.016356
[†] E _(g) / Hartree	-247.421615	-1278.419258	-1030.971388	-1278.326512	-969.600493	-722.153310	-969.506735	-1653.146775	-1405.701815	-1653.060361
*E _(g) COSMO / Hartree	-247.421966	-1278.419584	-1030.971504	-1278.327033	-969.601291	-722.153805	-969.507506	-1653.147908	-1405.702701	-1653.061166
Activity Coefficient-298K	2.451	6.892	61.442	13.321	4.859	8.111	15.241	1.846	9.192	25.545
Activity Coefficient-303K	2.486	7.514	64.456	14.203	4.762	8.107	14.769	1.973	9.469	27.315
Misfit Energy -298K / kcal mol-1	2.849	10.414	8.451	9.902	5.946	4.267	5.638	11.513	9.737	11.218
Misfit Energy -303K / kcal mol-1	2.896	10.524	8.527	10.016	6.054	4.338	5.742	11.688	9.887	11.371
Van der Waals Energy / kcal mol-1	-3.676	-10.544	-8.747	-10.569	-7.509	-5.567	-7.553	-13.312	-11.245	-11.795
	-	-	-	-	-	-	-	-	-	-
ΔG (kcal/mol) gas->solute-298K	155261.76557	802225.50951	646945.65260	802167.30145	608439.66274	453159.30325	608378.75297	1037376.78039	882097.04184	1037313.99110
	-	-	-	-	-	-	-	-	-	-
ΔG (kcal/mol) gas->solute-303K	155261.54869	802225.06323	646945.38459	802166.85958	608439.24479	453159.10781	608378.41244	1037376.06929	882096.55594	1037313.56873
ΔG (kcal/mol) liq->solute-298K	0.531	1.144	2.440	1.534	0.937	1.240	1.614	0.363	1.314	1.920
ΔG (kcal/mol) liq->solute-303K	0.549	1.215	2.510	1.599	0.940	1.261	1.622	0.410	1.354	1.992
μ gas-298K	155257.05099	802224.11084	646946.66155	802166.00749	608434.50915	453157.35865	608375.76472	1037371.38502	882095.46393	1037315.83360
μ gas-303K	155256.95511	802224.01495	646946.56567	802165.91160	608434.41326	453157.26277	608375.66884	1037371.28914	882095.36805	1037315.73772
μ pure-298K	-0.878	1.825	2.936	1.539	-1.723	1.183	-0.235	-1.391	1.475	4.290
μ pure-303K	-0.692	2.188	3.122	1.904	-1.321	1.345	0.085	-0.739	1.909	4.627
μ-infinite dilution-298K	-0.347	2.969	5.376	3.074	-0.786	2.423	1.379	-1.028	2.790	6.210
μ-infinite dilution-303K	-0.143	3.402	5.632	3.503	-0.381	2.606	1.707	-0.329	3.263	6.620
log vapor pressure -298K	-113804.714	-588032.305	-474212.468	-587989.924	-445986.314	-332165.380	-445942.163	-760398.602	-646578.599	-760353.718
log vapor pressure -303K	-111927.474	-578333.272	-466390.849	-578291.589	-438630.086	-326686.629	-438586.723	-747856.440	-635913.883	-747812.523

[†]Energy computed for COSMO optimized geometry
*Energy in COSMO solvent
AA=acrylamide; PX=product; RX=reactant;TS=transition state

	CapSH _(g)	CySH _(g)	GSH _(g)	CapSH _(aq)	CySH _(aq)	GSH _(aq)
Imaginary mode (i cm ⁻¹)	-1765.18	-1721.68	-1197.03	-1734.71	-1767.14	-1171.82
²⁹⁸ ΔG [‡] (kcal mol ⁻¹)	51.140	49.718	47.896	50.725	52.052	60.570
³⁰³ ΔG [‡] (kcal mol ⁻¹)	51.380	49.942	48.175	50.899	52.171	60.561
²⁹⁸ ΔH [‡] (kcal mol ⁻¹)	36.769	36.334	31.269	38.419	41.861	52.575
³⁰³ ΔH [‡] (kcal mol ⁻¹)	36.764	36.337	31.265	38.348	41.770	52.290
²⁹⁸ ΔS [‡] (cal mol ⁻¹ K ⁻¹)	-48.201	-44.891	-55.767	-41.274	-34.178	-26.814
³⁰³ ΔS [‡] (cal mol ⁻¹ K ⁻¹)	-48.216	-44.880	-55.780	-41.403	-34.310	-27.284
²⁹⁸ ΔG ^{React} (kcal mol ⁻¹)	-1.269	-1.824	-1.225	-2.773	-1.954	-1.147
³⁰³ ΔG ^{React} (kcal mol ⁻¹)	-1.031	-1.619	-1.068	-2.613	-1.720	-0.900