

Datos de la termodinámica de complejos Fe-A β

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Cuadro 1: Datos termodinámicos de los complejos Fe-A β estudiados para la formación de peróxido de hidrógeno mediante AscOH⁻ y O₂.

Δ Respecto a 20 + AscOH ⁻ + O ₂	M06L/cc-pVDZ					
	ΔE_g kcal/mol	ΔG_g kcal/mol	ΔH_g kcal/mol	ΔS_g kcal/mol	ΔG_{solv} kcal/mol	ΔG_r kcal/mol
21	-114.0	-97.1	-111.9	-14.8	91.2	-6.0
22	-98.7	-96.8	-98.6	-1.7	81.9	-14.9
23	59.9	62.0	58.3	-3.7	-36.6	25.4
24	-112.0	-95.0	-109.7	-14.7	91.5	-3.6
25	-106.3	-102.2	-106.0	-3.8	87.3	-14.9
26	67.4	64.9	62.6	-2.3	-42.2	22.7
27	14.7	-4.1	7.3	11.4	25.3	21.2
28	59.9	59.4	57.9	-1.5	-36.6	22.8
29	-62.4	-60.0	-73.6	-13.6	51.8	-8.2
30	12.2	0.8	10.0	9.2	-6.9	-6.0
31	-3.6	-12.4	-12.2	0.2	28.9	16.5
32	9.3	6.8	7.5	0.7	-1.7	5.1
33	-102.9	-88.2	-102.5	-14.3	84.8	-3.5
34	-86.3	-88.0	-87.3	0.7	80.0	-8.0
35	-67.8	-73.2	-62.3	10.9	37.0	-36.1
36	-104.2	-78.2	-102.1	-23.9	93.2	14.9
37	-95.4	-80.4	-94.9	-14.4	89.0	8.5