

	label	adj_list	Hf	Sf	Cp_300	Cp_1000
1	H2	1 H 0 {2,S} 2 H 0 {1,S}	0.00 kcal/mol	31.23 cal/(mol*K)	6.89 cal/(mol*K)	0.00 cal/(mol*K)
2	H	1 H 1	52.10 kcal/mol	27.42 cal/(mol*K)	4.97 cal/(mol*K)	52.10 cal/(mol*K)
3	O2	1 O 1 {2,S} 2 O 1 {1,S}	-0.00 kcal/mol	49.02 cal/(mol*K)	7.02 cal/(mol*K)	-0.00 cal/(mol*K)
4	OH	1 O 1	9.40 kcal/mol	43.91 cal/(mol*K)	7.14 cal/(mol*K)	9.40 cal/(mol*K)
5	CO3s1	1 C 0 {2,D} {3,S} {4,S} 2 O 0 {1,D} 3 O 0 {1,S} {4,S} 4 O 0 {1,S} {3,S}	-37.90 kcal/mol	61.28 cal/(mol*K)	11.82 cal/(mol*K)	-37.90 cal/(mol*K)