

2-Methylpropane

Low frequency normal modes:

29.	911.5	(E)	0.293
30.	778.6	(A1)	0.126
31.	445.0	(A1)	0.099
32.	367.2	(E)	0.022
33.	367.2	(E)	0.022
34.	240.8	(E)	0.000
35.	240.8	(E)	0.000
36.	210.8	(A2)	--

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 STATISTICAL THERMODYNAMICS ANALYSIS

Symmetry number : 3
 Optical isomers : 1
 Zero Point Energy : 79.756 Kcal/mol

	ENERGY (Kcal/mol)	ENTHALPY (Kcal/mol)	ENTROPY (eu)	FREE ENERGY (Kcal/mol)	HEAT CAPACITY
(cal/mol/deg)					
Translational	0.889	1.481	38.081	-9.873	4.967
Rotational	0.889	0.889	22.418	-5.795	2.980
Vibrational	81.612%	81.612%	9.796*	78.691%	14.610*
Potential	3.154#	3.154#	0.000	3.154#	0.000
Mixing	0.000	0.000	0.000	0.000	0.000
Total	86.543	87.136	70.295	66.177	22.558

FINAL STERIC ENERGY IS 3.1544 KCAL/MOL.
 HEAT OF FORMATION = -32.50

Propane

21.	960.8	(A2)	--
22.	938.0	(B1)	0.136
23.	850.2	(A1)	0.117
24.	802.7	(B2)	0.495
25.	379.3	(A1)	0.036
26.	250.6	(B2)	0.001
27.	208.1	(A2)	--

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 STATISTICAL THERMODYNAMICS ANALYSIS

	ENERGY (Kcal/mol)	ENTHALPY (Kcal/mol)	ENTROPY (eu)	FREE ENERGY (Kcal/mol)	HEAT CAPACITY
(cal/mol/deg)					
Translational	0.889	1.481	37.258	-9.627	4.967
Rotational	0.889	0.889	21.335	-5.472	2.980
Vibrational	63.539%	63.539%	5.822*	61.803%	9.103*
Potential	2.016#	2.016#	0.000	2.016#	0.000
Mixing	0.000	0.000	0.000	0.000	0.000
Total	67.331	67.924	64.415	48.718	17.051

FINAL STERIC ENERGY IS 2.0156 KCAL/MOL.
 HEAT OF FORMATION = -25.32