1,3-Dimethylbicyclo[1.1.0]butane

Inchi: InChI=1S/C6H10/c1-5-3-6(5,2)4-5/h3-4H2,1-2H3
InchiKey: IGAOOQCFXPSZTQ-UHFFFAOYSA-N
Formula: C6H10
SMILES: CC12CC1(C)C2
Mol. weight [g/mol]: 82.14
CAS: 930-25-6

Physical Properties

Property code	Value	Unit	Source
gf	134.36	kJ/mol	Joback Method
hf	21.23	kJ/mol	Joback Method
hfl	161.00 ± 4.20	kJ/mol	NIST Webbook
hfus	-0.83	kJ/mol	Joback Method
hvap	26.13	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.806		Crippen Method
mcvol	73.680	ml/mol	McGowan Method
pc	4480.21	kPa	Joback Method
tb	327.50 ± 1.00	K	NIST Webbook
tc	538.39	K	Joback Method
tf	248.10	K	Joback Method
vc	0.297	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	127.19	J/mol×K	342.10	Joback Method
cpg	142.52	J/mol×K	374.81	Joback Method
cpg	155.98	J/mol×K	407.53	Joback Method
cpg	167.77	J/mol×K	440.24	Joback Method
cpg	178.07	J/mol×K	472.96	Joback Method
cpg	187.08	J/mol×K	505.67	Joback Method
cpg	195.00	J/mol×K	538.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C930256&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume