Bicyclo[3.1.1]heptan-3-one, 6,6-dimethyl-2-(2-methylpropyl)-

Other names: 6,6-Dimethyl-2-(2-methylpropyl)-bicyclo[3.1.1]heptan-3-one (isomer)
Inchi: InChI=1S/C13H22O/c1-8(2)5-10-11-6-9(7-12(10)14)13(11,3)4/h8-11H,5-7H2,1-4H3
InchiKey: BLQUUSSRJOLJLD-UHFFFAOYSA-N
Formula: C13H22O
SMILES: CC(C)CC1C(=O)CC2CC1C2(C)C
Mol. weight [g/mol]: 194.31

Physical Properties

Property code	Value	Unit	Source
gf	22.04	kJ/mol	Joback Method
hf	-340.63	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.284		Crippen Method
mcvol	173.880	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1237.00		NIST Webbook
tb	572.87	K	Joback Method
tc	789.25	K	Joback Method
tf	337.27	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.83	J/mol×K	572.87	Joback Method
cpg	493.81	J/mol×K	608.93	Joback Method
cpg	513.61	J/mol×K	645.00	Joback Method
cpg	532.35	J/mol×K	681.06	Joback Method
cpg	550.16	J/mol×K	717.12	Joback Method
cpg	567.16	J/mol×K	753.18	Joback Method
cpg	583.47	J/mol×K	789.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U163979&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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume