1,6,6-trimethylbicyclo[3.3.0]octan-3-one

Inchi: InChI=1S/C11H18O/c1-10(2)4-5-11(3)7-8(12)6-9(10)11/h9H,4-7H2,1-3H3
InchiKey: BYBQDPBXNGMTFY-UHFFFAOYSA-N
Formula: C11H18O
SMILES: CC1(C)CCC2(C)CC(=O)CC12
Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
gf	-2.24	kJ/mol	Joback Method
hf	-264.65	kJ/mol	Joback Method
hfus	4.30	kJ/mol	Joback Method
hvap	41.89	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.792		Crippen Method
mcvol	145.700	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1454.00		NIST Webbook
tb	536.73	K	Joback Method
tc	773.98	K	Joback Method
tf	354.35	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.99	J/mol×K	536.73	Joback Method
cpg	391.94	J/mol×K	576.27	Joback Method
cpg	410.48	J/mol×K	615.81	Joback Method
cpg	427.85	J/mol×K	655.36	Joback Method
cpg	444.34	J/mol×K	694.90	Joback Method
cpg	460.19	J/mol×K	734.44	Joback Method
cpg	475.69	J/mol×K	773.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R423226&Units=SI

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