1,3,4,5,5,6-Hexamethylbicyclo[3.1.0]hex-3-en-2-on

Inchi: InChI=1S/C12H18O/c1-7-8(2)11(5)10(3,4)12(11,6)9(7)13/h1-6H3
InchiKey: SONHFFYISNVFJL-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CC1=C(C)C2(C)C(C)(C)C2(C)C1=O
Mol. weight [g/mol]: 178.27
CAS: 2206-69-1

Physical Properties

Property code	Value	Unit	Source
gf	35.59	kJ/mol	Joback Method
hf	-222.89	kJ/mol	Joback Method
hfus	5.24	kJ/mol	Joback Method
hvap	44.23	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.958		Crippen Method
mcvol	155.490	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
tb	560.43	K	Joback Method
tc	790.42	K	Joback Method
tf	422.36	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.04	J/mol×K	560.43	Joback Method
cpg	415.26	J/mol×K	598.76	Joback Method
cpg	430.42	J/mol×K	637.09	Joback Method
cpg	444.88	J/mol×K	675.43	Joback Method
cpg	458.99	J/mol×K	713.76	Joback Method
cpg	473.10	J/mol×K	752.09	Joback Method
cpg	487.57	J/mol×K	790.42	Joback Method

Sources

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=C2206691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume