6-Oxobornyl acetate

Inchi: InChI=1S/C12H18O3/c1-7(13)15-10-6-8-5-9(14)12(10,4)11(8,2)3/h8,10H,5-6H2,1-4H3/t8
InchiKey: QJQUXQNTQQVERR-BSTRBVHOSA-N
Formula: C12H18O3
SMILES: CC(=O)OC1CC2CC(=O)C1(C)C2(C)C
Mol. weight [g/mol]: 210.27

Physical Properties

Property code	Value	Unit	Source
gf	-223.35	kJ/mol	Joback Method
hf	-544.27	kJ/mol	Joback Method
hfus	12.85	kJ/mol	Joback Method
hvap	52.79	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.943		Crippen Method
mcvol	167.230	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
tb	626.96	K	Joback Method
tc	855.74	K	Joback Method
tf	437.06	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.05	J/mol×K	626.96	Joback Method
cpg	488.81	J/mol×K	665.09	Joback Method
cpg	505.75	J/mol×K	703.22	Joback Method
cpg	522.09	J/mol×K	741.35	Joback Method
cpg	538.07	J/mol×K	779.48	Joback Method
cpg	553.88	J/mol×K	817.61	Joback Method
cpg	569.77	J/mol×K	855.74	Joback Method

Sources

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=R341565&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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