6-hydroxy-Isobornyl Isobutyrate

Inchi: InChI=1S/C15H26O2/c1-9(2)13(16)17-12-8-11-7-10(3)15(12,6)14(11,4)5/h9-12H,7-8H2,1
InchiKey: GPEHIMRFBMDMNN-JTHFCNIQSA-N
Formula: C15H26O2
SMILES: CC(C)C(=O)OC1CC2CC(C)C1(C)C2(C)C
Mol. weight [g/mol]: 238.37
CAS: 107783-32-4

Physical Properties

Property code	Value	Unit	Source
gf	-85.65	kJ/mol	Joback Method
hf	-494.11	kJ/mol	Joback Method
hfus	18.66	kJ/mol	Joback Method
hvap	54.52	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.646		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	1602.00		NIST Webbook
rinpol	1638.00		NIST Webbook
tb	622.67	K	Joback Method
tc	832.09	K	Joback Method
tf	383.41	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.87	J/mol×K	622.67	Joback Method
cpg	615.65	J/mol×K	657.57	Joback Method
cpg	635.42	J/mol×K	692.48	Joback Method
cpg	654.38	J/mol×K	727.38	Joback Method
cpg	672.74	J/mol×K	762.28	Joback Method
cpg	690.68	J/mol×K	797.19	Joback Method
cpg	708.41	J/mol×K	832.09	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=C107783324&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