

5-hydroxy-isobornyl butyrate

Inchi:	InChI=1S/C14H24O3/c1-5-6-12(16)17-11-7-9-10(15)8-14(11,4)13(9,2)3/h9-11,15H,5-8H2
InchiKey:	ZGBYUSKULPTYKK-DGVZPSOQSA-N
Formula:	C14H24O3
SMILES:	CCCC(=O)OC1CC2C(O)CC1(C)C2(C)C
Mol. weight [g/mol]:	240.34

Physical Properties

Property code	Value	Unit	Source
gf	-228.45	kJ/mol	Joback Method
hf	-620.42	kJ/mol	Joback Method
hfus	23.68	kJ/mol	Joback Method
hvap	69.36	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.515		Crippen Method
mcvol	199.710	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1661.00		NIST Webbook
tb	692.41	K	Joback Method
tc	888.83	K	Joback Method
tf	447.96	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.43	J/mol×K	692.41	Joback Method
cpg	626.22	J/mol×K	725.15	Joback Method
cpg	642.53	J/mol×K	757.88	Joback Method
cpg	658.50	J/mol×K	790.62	Joback Method
cpg	674.30	J/mol×K	823.36	Joback Method
cpg	690.10	J/mol×K	856.09	Joback Method
cpg	706.06	J/mol×K	888.83	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=R507116&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
hvac:	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

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