Bornyl butyrate

Other names:	Isobornyl butyrate
	Isobornyl butanoate
	Bornyl butanoate
	exo-bornyl butyrate
Inchi:	InChI=1S/C14H24O2/c1-5-6-12(15)16-11-9-10-7-8-14(11,4)13(10,2)3/h10-11H,5-9H2,1-4
InchiKey:	VIPNQHBVIDJXJE-UHIISALHSA-N
Formula:	C14H24O2
SMILES:	CCCC(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]:	224.34
CAS:	58479-55-3

Physical Properties

Property code	Value	Unit	Source
gf	-83.92	kJ/mol	Joback Method
hf	-447.85	kJ/mol	Joback Method
hfus	18.52	kJ/mol	Joback Method
hvap	52.99	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.545		Crippen Method
mcvol	193.840	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1463.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1473.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1760.00		NIST Webbook
tb	604.90	K	Joback Method
tc	813.55	K	Joback Method
tf	391.38	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.99	J/mol×K	604.90	Joback Method
cpg	559.47	J/mol×K	639.68	Joback Method
cpg	577.93	J/mol×K	674.45	Joback Method
cpg	595.57	J/mol×K	709.23	Joback Method
cpg	612.59	J/mol×K	744.00	Joback Method
cpg	629.20	J/mol×K	778.78	Joback Method
cpg	645.60	J/mol×K	813.55	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=C58479553&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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