

BORNYL BUTYRATE

Other names:	Bornyl butanoate Isobornyl butanoate Isobornyl butyrate 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,5-9H2,1-4H
InchiKey:	VIPNQHBVIDJXJE-UHIIISALHSA-N
Formula:	C14H24O2
SMILES:	CCCC(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]:	224.34

Physical Properties

Property code	Value	Unit	Source
hf	-503.46	kJ/mol	Cheméo Relay (1.0)
hfus	18.52	kJ/mol	Joback Method
hvap	69.39	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.67		Cheméo Relay (1.0)
logp	3.545		Crippen Method
mcvol	193.840	ml/mol	McGowan Method
tb	518.51	K	Cheméo Relay (1.0)
tf	342.76	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13109701&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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