

Butanoic acid, 1,7,7-trimethylbicyclo[2.2.1]hept-2-yl ester, endo-

Other names:	Butyric acid, 2-bornyl ester Bornyl ester of n-butanoic acid Borneol, butyrate Bornyl butyrate Bornyl butanoate endo-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,5-9H2,1-4H3
InchiKey:	VIPNQHBVIDJXJE-UHFFFAOYSA-N
Formula:	C14H24O
SMILES:	CCCC(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]:	208.34
CAS:	13109-70-1

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	1451.00		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	629.20	J/mol×K	778.78	Joback Method
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	645.60	J/mol×K	813.55	Joback Method
hvapt	59.60	kJ/mol	433.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13109701&Units=SI
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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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