

Bornyl isovalerate

Other names:	Butanoic acid, 3-methyl-, (1R,2S,4R)-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl ester, ^{rel-} Bornyval Hysterol Isovaleric acid, 2-bornyl ester, endo- 2-Bornyl 3-methylbutyrate Bornyl ester of isopentanoic acid Borneol, isovalerate 1,7,7-Trimethylbicyclo[2.2.1]hept-2-yl 3-methylbutanoate, endo- Bornyl 3-methylbutanoate Butanoic acid, 3-methyl-, 1,7,7-trimethylbicyclo[2.2.1]hept-2-yl ester, endo- Isovaleric acid, 2-bornyl ester NSC 68007 endo-bornyl isovalerate
Inchi:	InChI=1S/C15H26O2/c1-10(2)8-13(16)17-12-9-11-6-7-15(12,5)14(11,3)4/h10-12H,6-9H2
InchiKey:	MPYYVGIJHREDBO-MQYJIDSJSA-N
Formula:	C15H26O2
SMILES:	CC(C)CC(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]:	238.37
CAS:	76-50-6

Physical Properties

Property code	Value	Unit	Source
gf	-77.94	kJ/mol	Joback Method
hf	-473.77	kJ/mol	Joback Method
hfus	17.59	kJ/mol	Joback Method
hvap	54.83	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.790		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1492.00		NIST Webbook

rinpol	1501.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1488.00		NIST Webbook
ripol	1774.00		NIST Webbook
ripol	1774.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1753.00		NIST Webbook
tb	627.34	K	Joback Method
tc	836.82	K	Joback Method
tf	387.65	K	Joback Method
vc	0.793	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.55	J/mol×K	627.34	Joback Method
cpg	613.85	J/mol×K	662.25	Joback Method
cpg	633.16	J/mol×K	697.17	Joback Method
cpg	651.71	J/mol×K	732.08	Joback Method
cpg	669.68	J/mol×K	766.99	Joback Method
cpg	687.30	J/mol×K	801.90	Joback Method
cpg	704.76	J/mol×K	836.82	Joback Method

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C76506&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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