

Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, acetate, (1S-endo)-

Other names: Borneol, acetate, (1S,2R,4S)-(-)-

(-)-Bornyl acetate

L-«alpha»-bornyl acetate

L-bornyl acetate

Levo-bornyl acetate

L-born-2-yl acetate

Inchi: InChI=1S/C12H20O2/c1-8(13)14-10-7-9-5-6-12(10,4)11(9,2)3/h9-10H,5-7H2,1-4H3/t9-,1

InchiKey: KGEKLUUHTZCSIP-SCVCMEIPSA-N

Formula: C12H20O2

SMILES: CC(=O)OC1CC2CCC1(C)C2(C)C

Mol. weight [g/mol]: 196.29

CAS: 5655-61-8

Physical Properties

Property code	Value	Unit	Source
gf	-100.76	kJ/mol	Joback Method
hf	-406.57	kJ/mol	Joback Method
hfus	13.34	kJ/mol	Joback Method
hvap	48.54	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.764		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1285.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1284.00		NIST Webbook
tb	496.70	K	NIST Webbook
tc	774.82	K	Joback Method
tf	368.84	K	Joback Method
vc	0.631	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.90	J/mol×K	559.14	Joback Method
cpg	456.54	J/mol×K	595.09	Joback Method
cpg	474.00	J/mol×K	631.03	Joback Method
cpg	490.47	J/mol×K	666.98	Joback Method
cpg	506.18	J/mol×K	702.93	Joback Method
cpg	521.34	J/mol×K	738.88	Joback Method
cpg	536.18	J/mol×K	774.82	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5655618&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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