Isobornyl acetate

Other names:	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, acetate, exo-
	Isoborneol, acetate
	Acetic acid, isobornyl ester
	Pichtosin
	Pichtosine
	Bicyclo(2.2.1)heptan-2-ol, 1,7,7-trimethyl-, 2-acetate, (1R,2R,4R)-rel-
	exo-Bornyl acetate
	2-Bornyl acetate, exo-
	exo-1,7,7-Trimethylbicyclo(2.2.1)hept-2-yl acetate
	endo-Bornyl acetate
	(+)-Bornyl acetate = Isobornyl 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-SQLBVSGCSA-N
Formula:	C12H20O2
SMILES:	CC(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]:	196.29
CAS:	125-12-2

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	1288.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1304.00		NIST Webbook

rinpol	1270.00	NIST Webbook
rinpol	1277.00	NIST Webbook
rinpol	1285.00	NIST Webbook
rinpol	1302.00	NIST Webbook
rinpol	1286.00	NIST Webbook
rinpol	1268.00	NIST Webbook
rinpol	1279.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1285.00	NIST Webbook
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ripol	1571.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1613.00		NIST Webbook
tb	559.14	K	Joback Method
tc	774.82	K	Joback Method
tf	368.84	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.34	J/mol×K	738.88	Joback Method
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	536.18	J/mol×K	774.82	Joback Method
hvapt	56.10	kJ/mol	427.00	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C125122&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
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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