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	1278.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1286.00		NIST Webbook

rinpol	1268.00	NIST Webbook
rinpol	1290.00	NIST Webbook
rinpol	1283.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1294.00	NIST Webbook
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ripol	1549.00		NIST Webbook
ripol	1554.00		NIST Webbook
ripol	1625.00		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	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
hvapt	56.10	kJ/mol	427.00	NIST Webbook

Sources

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=C125122&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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