Isobornyl propionate

Other names:	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, propanoate, exo- Isoborneol, propionate iso-Bornyl n-propionate exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl propionate
Inchi:	InChI=1S/C13H22O2/c1-5-11(14)15-10-8-9-6-7-13(10,4)12(9,2)3/h9-10H,5-8H2,1-4H3/t9
InchiKey:	FAFMZORPAAGQFV-RUETXSTFSA-N
Formula:	C13H22O2
SMILES:	CCC(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]:	210.31
CAS:	2756-56-1

Physical Properties

Property code	Value	Unit	Source
gf	-92.34	kJ/mol	Joback Method
hf	-427.21	kJ/mol	Joback Method
hfus	15.93	kJ/mol	Joback Method
hvap	50.77	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.154		Crippen Method
mcvol	179.750	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1388.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1384.00		NIST Webbook
ripol	1676.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1681.00		NIST Webbook
tb	582.02	K	Joback Method
tc	794.09	K	Joback Method
tf	380.11	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.22	J/mol×K	582.02	Joback Method
cpg	507.29	J/mol×K	617.37	Joback Method
cpg	525.26	J/mol×K	652.71	Joback Method
cpg	542.34	J/mol×K	688.06	Joback Method
cpg	558.72	J/mol×K	723.40	Joback Method
cpg	574.62	J/mol×K	758.75	Joback Method
cpg	590.26	J/mol×K	794.09	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2756561&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume