

isobornyl propanoate

Inchi:	InChI=1S/C12H20O2/c1-4-11(13)14-10-7-8-5-6-9(10)12(8,2)3/h8-10H,4-7H2,1-3H3/t8?,9
InchiKey:	ZMTXIFSFOZCIJW-UDNWOFFPSA-N
Formula:	C12H20O2
SMILES:	CCC(=O)OC1CC2CCC1C2(C)C
Mol. weight [g/mol]:	196.29

Physical Properties

Property code	Value	Unit	Source
gf	-95.27	kJ/mol	Joback Method
hf	-421.81	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	49.69	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.764		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1382.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1349.00		NIST Webbook
rinpol	1349.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1382.00		NIST Webbook
tb	558.90	K	Joback Method
tc	766.28	K	Joback Method
tf	344.94	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.95	J/mol×K	558.90	Joback Method
cpg	457.77	J/mol×K	593.46	Joback Method
cpg	475.48	J/mol×K	628.03	Joback Method

cpg	492.21	J/mol×K	662.59	Joback Method
cpg	508.06	J/mol×K	697.15	Joback Method
cpg	523.16	J/mol×K	731.72	Joback Method
cpg	537.62	J/mol×K	766.28	Joback Method

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=R82786&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
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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