Isobornyl angelate

Inchi: InChI=1S/C14H22O2/c1-5-9(2)13(15)16-12-8-10-6-7-11(12)14(10,3)4/h5,10-12H,6-8H2,1
InchiKey: OBPZMFLAYLWFTO-ZKYAPIFESA-N
Formula: C14H22O2
SMILES: CC=C(C)C(=O)OC1CC2CCC1C2(C)C
Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	-6.76	kJ/mol	Joback Method
hf	-355.66	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	54.18	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.320		Crippen Method
mcvol	189.540	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
rinpol	1592.00		NIST Webbook
tb	608.70	K	Joback Method
tc	821.81	K	Joback Method
tf	348.44	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.05	J/mol×K	608.70	Joback Method
cpg	541.61	J/mol×K	644.22	Joback Method
cpg	560.05	J/mol×K	679.74	Joback Method
cpg	577.51	J/mol×K	715.25	Joback Method
cpg	594.15	J/mol×K	750.77	Joback Method
cpg	610.11	J/mol×K	786.29	Joback Method
cpg	625.53	J/mol×K	821.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R514802&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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