

Bornyl angelate

Inchi:	InChI=1S/C15H24O2/c1-6-10(2)13(16)17-12-9-11-7-8-15(12,5)14(11,3)4/h6,11-12H,7-9H
InchiKey:	ZUVAGNOBOHVXJJ-WZDSXNDXSA-N
Formula:	C15H24O2
SMILES:	CC=C(C)C(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]:	236.35

Physical Properties

Property code	Value	Unit	Source
gf	-3.83	kJ/mol	Joback Method
hf	-361.06	kJ/mol	Joback Method
hfus	20.00	kJ/mol	Joback Method
hvap	55.26	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.711		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	1547.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1547.00		NIST Webbook
tb	631.82	K	Joback Method
tc	849.20	K	Joback Method
tf	383.61	K	Joback Method
vc	0.780	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.31	J/mol×K	631.82	Joback Method
cpg	592.10	J/mol×K	668.05	Joback Method
cpg	610.91	J/mol×K	704.28	Joback Method

cpg	628.99	J/mol×K	740.51	Joback Method
cpg	646.59	J/mol×K	776.74	Joback Method
cpg	663.95	J/mol×K	812.97	Joback Method
cpg	681.31	J/mol×K	849.20	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=R204387&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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