

6-Hydroxyhumulene epoxide

Inchi:	InChI=1S/C15H26O2/c1-11-6-5-8-14(2,3)10-13-15(4,17-13)9-7-12(11)16/h5,8,11-13,16H
InchiKey:	GZRATLUSAGGRAW-VMPITWQZSA-N
Formula:	C15H26O2
SMILES:	CC1CC=CC(C)(C)CC2OC2(C)CCC1O
Mol. weight [g/mol]:	238.37

Physical Properties

Property code	Value	Unit	Source
gf	-102.77	kJ/mol	Joback Method
hf	-501.28	kJ/mol	Joback Method
hfus	22.18	kJ/mol	Joback Method
hvap	68.09	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.297		Crippen Method
mvol	207.930	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1753.00		NIST Webbook
rinpol	1753.00		NIST Webbook
tb	686.46	K	Joback Method
tc	904.64	K	Joback Method
tf	396.80	K	Joback Method
vc	0.760	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.20	J/molxK	686.46	Joback Method
cpg	657.41	J/molxK	722.82	Joback Method
cpg	677.73	J/molxK	759.19	Joback Method
cpg	697.38	J/molxK	795.55	Joback Method
cpg	716.55	J/molxK	831.91	Joback Method
cpg	735.46	J/molxK	868.28	Joback Method
cpg	754.30	J/molxK	904.64	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R628807&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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