Humulene diepoxide A

Inchi: InChI=1S/C15H24O2/c1-13(2)7-5-8-14(3)11(16-14)6-9-15(4)12(10-13)17-15/h5,7,11-12H
InchiKey: UFBUQKAQYQDEOE-SJFFUCJWSA-N
Formula: C15H24O2
SMILES: CC1(C)C=CCC2(C)OC2CCC2(C)OC2C1
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	35.10	kJ/mol	Joback Method
hf	-360.35	kJ/mol	Joback Method
hfus	21.04	kJ/mol	Joback Method
hvap	54.65	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.458		Crippen Method
mcvol	197.070	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
ripol	2356.00		NIST Webbook
ripol	2340.00		NIST Webbook
ripol	2340.00		NIST Webbook
ripol	2358.00		NIST Webbook
ripol	2362.00		NIST Webbook
tb	624.34	K	Joback Method
tc	868.62	K	Joback Method
tf	415.67	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.02	J/mol×K	624.34	Joback Method
cpg	598.00	J/mol×K	665.05	Joback Method
cpg	619.71	J/mol×K	705.77	Joback Method
cpg	640.64	J/mol×K	746.48	Joback Method
cpg	661.26	J/mol×K	787.19	Joback Method

cpg	682.04	J/mol×K	827.90	Joback Method
cpg	703.47	J/mol×K	868.62	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=R492965&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume