Humulene 1,2-epoxide

Inchi: InChI=1S/C15H24O/c1-11-6-5-7-12(2)10-13-14(16-13)15(3,4)9-8-11/h7-8,13-14H,5-6,9-1
InchiKey: WSIKWSKUPSHZMF-NFLJZBCPSA-N
Formula: C15H24O
SMILES: CC1=CCC(C)(C)C2OC2CC(C)=CCC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	65.66	kJ/mol	Joback Method
hf	-288.77	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	54.80	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.247		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	1615.00		NIST Webbook
tb	612.50	K	Joback Method
tc	844.62	K	Joback Method
tf	346.36	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.86	J/mol×K	612.50	Joback Method
cpg	564.13	J/mol×K	651.19	Joback Method
cpg	586.01	J/mol×K	689.87	Joback Method
cpg	606.64	J/mol×K	728.56	Joback Method
cpg	626.16	J/mol×K	767.25	Joback Method
cpg	644.71	J/mol×K	805.93	Joback Method
cpg	662.44	J/mol×K	844.62	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R614076&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume