Humulene epoxide III

Other names: Humulene epoxide 3
Inchi: InChI=1S/C15H24O/c1-12-6-7-13-15(4,16-13)10-5-9-14(2,3)11-8-12/h5,8-9,13H,6-7,10-1
InchiKey: QTGAEXCCAPTGLB-ZYEZJADKSA-N
Formula: C15H24O
SMILES: CC1=CCC(C)(C)C=CCC2(C)OC2CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	69.80	kJ/mol	Joback Method
hf	-262.06	kJ/mol	Joback Method
hfus	16.79	kJ/mol	Joback Method
hvap	52.99	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.247		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
ripol	2081.00		NIST Webbook
ripol	2081.00		NIST Webbook
ripol	2081.00		NIST Webbook
ripol	2081.00		NIST Webbook
ripol	2081.00		NIST Webbook
ripol	2081.00		NIST Webbook
ripol	2081.00		NIST Webbook
ripol	2083.00		NIST Webbook
ripol	2049.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2081.00		NIST Webbook
ripol	2081.00		NIST Webbook
tb	607.76	K	Joback Method
tc	848.30	K	Joback Method
tf	357.74	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.18	J/mol×K	607.76	Joback Method
cpg	561.67	J/mol×K	647.85	Joback Method
cpg	583.74	J/mol×K	687.94	Joback Method
cpg	604.67	J/mol×K	728.03	Joback Method
cpg	624.76	J/mol×K	768.12	Joback Method
cpg	644.27	J/mol×K	808.21	Joback Method
cpg	663.49	J/mol×K	848.30	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R229391&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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume