«alpha»-Humulene epoxide II

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-PIHCAMFYSA-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	1606.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1606.00		NIST Webbook
ripol	2009.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R204634&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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