1,2-Epoxyhumulene

Other names: humulene epoxide-II
Inchi: InChI=1S/C15H26O/c1-12-7-5-9-14(2,3)11-13-15(4,16-13)10-6-8-12/h5,9,12-13H,6-8,10-
InchiKey: MNJMQINRKGQYTP-WEVVVXLNSA-N
Formula: C15H26O
SMILES: CC1CC=CC(C)(C)CC2OC2(C)CCC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	41.76	kJ/mol	Joback Method
hf	-328.71	kJ/mol	Joback Method
hfus	17.02	kJ/mol	Joback Method
hvap	51.72	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.326		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	1608.00		NIST Webbook
ripol	2071.00		NIST Webbook
ripol	2071.00		NIST Webbook
tb	598.95	K	Joback Method
tc	836.23	K	Joback Method
tf	340.22	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.62	J/mol×K	598.95	Joback Method
cpg	585.13	J/mol×K	638.50	Joback Method
cpg	609.08	J/mol×K	678.04	Joback Method
cpg	631.73	J/mol×K	717.59	Joback Method
cpg	653.35	J/mol×K	757.13	Joback Method
cpg	674.21	J/mol×K	796.68	Joback Method

cpg	694.58	J/mol×K	836.23	Joback Method

Sources

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=R229955&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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