Caryophyllene, 5,6-epoxide

Inchi: InChI=1S/C15H22O/c1-9-5-6-12-11(8-15(12,3)4)10(2)7-13-14(9)16-13/h5,11-14H,2,6-8H
InchiKey: NXKCYZMFPBDBKQ-KRKYHIKISA-N
Formula: C15H22O
SMILES: C=C1CC2OC2C(C)=CCC2C1CC2(C)C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	187.75	kJ/mol	Joback Method
hf	-179.90	kJ/mol	Joback Method
hfus	26.21	kJ/mol	Joback Method
hvap	53.09	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.712		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1571.00		NIST Webbook
ripol	1953.00		NIST Webbook
tb	596.78	K	Joback Method
tc	820.63	K	Joback Method
tf	371.02	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.09	J/mol×K	596.78	Joback Method
cpg	542.87	J/mol×K	634.09	Joback Method
cpg	563.28	J/mol×K	671.40	Joback Method
cpg	582.52	J/mol×K	708.70	Joback Method
cpg	600.74	J/mol×K	746.01	Joback Method
cpg	618.14	J/mol×K	783.32	Joback Method
cpg	634.88	J/mol×K	820.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R545767&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