Cariophyllene oxide II

Inchi: InChI=1S/C15H24O/c1-10-5-6-13-15(4,16-13)8-7-12-11(10)9-14(12,2)3/h11-13H,1,5-9H2
InchiKey: NVEQFIOZRFFVFW-YKQCJFHZSA-N
Formula: C15H24O
SMILES: C=C1CCC2OC2(C)CCC2C1CC2(C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	161.93	kJ/mol	Joback Method
hf	-210.97	kJ/mol	Joback Method
hfus	19.08	kJ/mol	Joback Method
hvap	50.99	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.936		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
ripol	2008.00		NIST Webbook
ripol	2008.00		NIST Webbook
tb	592.88	K	Joback Method
tc	822.50	K	Joback Method
tf	381.64	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.37	J/mol×K	592.88	Joback Method
cpg	562.46	J/mol×K	631.15	Joback Method
cpg	584.07	J/mol×K	669.42	Joback Method
cpg	604.52	J/mol×K	707.69	Joback Method
cpg	624.09	J/mol×K	745.96	Joback Method
cpg	643.08	J/mol×K	784.23	Joback Method
cpg	661.78	J/mol×K	822.50	Joback Method

Sources

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=R616314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume