(+) Caryophyllene oxide

Other names: (-)-Caryophyllene oxide
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-UHFFFAOYSA-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
rinpol	1542.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
ripol	1966.00		NIST Webbook
ripol	1990.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1966.00		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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R332402&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