1,8-Epoxycadin-4-ene

Inchi: InChI=1S/C15H24O/c1-9(2)12-8-14-11(4)15(16-14)6-5-10(3)7-13(12)15/h7,9,11-14H,5-6
InchiKey: DWHKMTZSGDMQER-VIGLNQMMSA-N
Formula: C15H24O
SMILES: CC1=CC2C(C(C)C)CC3OC2(CC1)C3C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	144.33	kJ/mol	Joback Method
hf	-263.26	kJ/mol	Joback Method
hfus	25.94	kJ/mol	Joback Method
hvap	52.37	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.792		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1550.00		NIST Webbook
tb	592.91	K	Joback Method
tc	812.06	K	Joback Method
tf	345.86	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.04	J/mol×K	592.91	Joback Method
cpg	563.43	J/mol×K	629.43	Joback Method
cpg	584.42	J/mol×K	665.96	Joback Method
cpg	604.18	J/mol×K	702.48	Joback Method
cpg	622.90	J/mol×K	739.01	Joback Method
cpg	640.76	J/mol×K	775.53	Joback Method
cpg	657.94	J/mol×K	812.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232921&Units=SI

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