10,11-Epoxy calamenene

Inchi: InChI=1S/C15H20O/c1-10-5-6-13-11(9-10)12-7-8-15(13,4)16-14(12,2)3/h5-6,9,12H,7-8H
InchiKey: RWNMGACJGXHHHN-CVRLYYSRSA-N
Formula: C15H20O
SMILES: Cc1ccc2c(c1)C1CCC2(C)OC1(C)C
Mol. weight [g/mol]: 216.32

Physical Properties

Property code	Value	Unit	Source
gf	185.26	kJ/mol	Joback Method
hf	-115.60	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	54.31	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.896		Crippen Method
mcvol	182.600	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	1485.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1476.00		NIST Webbook
tb	615.48	K	Joback Method
tc	852.68	K	Joback Method
tf	416.28	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.08	J/mol×K	615.48	Joback Method
cpg	514.95	J/mol×K	655.01	Joback Method
cpg	532.70	J/mol×K	694.55	Joback Method
cpg	549.68	J/mol×K	734.08	Joback Method
cpg	566.21	J/mol×K	773.61	Joback Method
cpg	582.64	J/mol×K	813.15	Joback Method
cpg	599.28	J/mol×K	852.68	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=R229737&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