6,7;7,10-Bisepoxy-6,7-seco-calamenene

Other names: 6,7-Bisepoxy-sec-calamenene
Inchi: InChI=1S/C15H20O2/c1-10(2)15-8-7-14(4,17-15)12-6-5-11(3)9-13(12)16-15/h5-6,9-10H,
InchiKey: ZOYQOKPXTQBYKL-UHFFFAOYSA-N
Formula: C15H20O2
SMILES: Cc1ccc2c(c1)OC1(C(C)C)CCC2(C)O1
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	104.41	kJ/mol	Joback Method
hf	-232.54	kJ/mol	Joback Method
hfus	23.98	kJ/mol	Joback Method
hvap	58.74	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.765		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1580.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1588.00		NIST Webbook
ripol	2109.00		NIST Webbook
ripol	2049.00		NIST Webbook
ripol	2109.00		NIST Webbook
ripol	2049.00		NIST Webbook
tb	646.66	K	Joback Method
tc	885.53	K	Joback Method
tf	432.09	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.22	J/mol×K	646.66	Joback Method

cpg	544.11	J/mol×K	686.47	Joback Method
cpg	561.13	J/mol×K	726.28	Joback Method
cpg	577.62	J/mol×K	766.09	Joback Method
cpg	593.93	J/mol×K	805.91	Joback Method
cpg	610.41	J/mol×K	845.72	Joback Method
cpg	627.40	J/mol×K	885.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229544&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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