

Calamenene-1,11-epoxide

Other names:	1,10-Oxidocalamenene
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-WFASDCNBSA-N
Formula:	C15H20O
SMILES:	<chem>Cc1ccc2c(c1)C1CCC2(C)OC1(C)C</chem>
Mol. weight [g/mol]:	216.32
CAS:	143785-42-6

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	1491.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1491.00		NIST Webbook
ripol	1900.00		NIST Webbook
tb	615.48	K	Joback Method
tc	852.68	K	Joback Method
tf	416.28	K	Joback Method
vc	0.698	m ³ /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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C143785426&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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