7,10-Epoxy-2,6,10-trimethyl-dodeca-2,11-dien-6-ol

B

Inchi: InChI=1S/C15H26O2/c1-6-14(4)11-9-13(17-14)15(5,16)10-7-8-12(2)3/h6,8,13,16H,1,7,9-

InchiKey: OIVTVPOJCWXSIC-UHFFFAOYSA-N

Formula: C15H26O2

SMILES: C=CC1(C)CCC(C(C)(O)CCC=C(C)C)O1

Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	38.18	kJ/mol	Joback Method
hf	-357.67	kJ/mol	Joback Method
hfus	25.58	kJ/mol	Joback Method
hvap	67.04	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.608		Crippen Method
mcvol	214.490	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	1555.00		NIST Webbook
ripol	1985.00		NIST Webbook
tb	670.07	K	Joback Method
tc	868.36	K	Joback Method
tf	358.38	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.27	J/mol×K	670.07	Joback Method
cpg	636.72	J/mol×K	703.12	Joback Method
cpg	653.31	J/mol×K	736.17	Joback Method
cpg	669.17	J/mol×K	769.22	Joback Method
cpg	684.44	J/mol×K	802.26	Joback Method
cpg	699.24	J/mol×K	835.31	Joback Method
cpg	713.72	J/mol×K	868.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229559&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