6,9-Epoxyfarnesa-1,7(14),10-trien-3-ol

Inchi: InChI=1S/C15H24O2/c1-6-15(5,16)8-7-14-12(4)10-13(17-14)9-11(2)3/h6,9,13-14,16H,1,4
InchiKey: LJPFBTWRZZGKFP-UHFFFAOYSA-N
Formula: C15H24O2
SMILES: C=CC(C)(O)CCC1OC(C=C(C)C)CC1=C
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	96.75	kJ/mol	Joback Method
hf	-288.67	kJ/mol	Joback Method
hfus	30.72	kJ/mol	Joback Method
hvap	68.35	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.383		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
rinpol	1601.00		NIST Webbook
rinpol	1600.00		NIST Webbook
ripol	2257.00		NIST Webbook
ripol	2262.00		NIST Webbook
tb	668.99	K	Joback Method
tc	862.55	K	Joback Method
tf	348.16	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.85	J/mol×K	668.99	Joback Method
cpg	615.48	J/mol×K	701.25	Joback Method
cpg	631.15	J/mol×K	733.51	Joback Method
cpg	645.92	J/mol×K	765.77	Joback Method
cpg	659.85	J/mol×K	798.03	Joback Method
cpg	672.99	J/mol×K	830.29	Joback Method

cpg	685.41	J/mol×K	862.55	Joback Method

Sources

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=R232510&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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