3,6;6,9-Bisepoxyfarnesa-1,7(14),10-triene

Other names: 3,6,6,9-Bisepoxy-farnesa-1,7(14),10-triene
Inchi: InChI=1S/C15H22O2/c1-6-14(5)7-8-15(17-14)12(4)10-13(16-15)9-11(2)3/h6,9,13H,1,4,7-
InchiKey: WKVFNUBTMXSGNM-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: C=CC1(C)CCC2(OC(C=C(C)C)CC2=C)O1
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	182.28	kJ/mol	Joback Method
hf	-162.57	kJ/mol	Joback Method
hfus	25.46	kJ/mol	Joback Method
hvap	55.26	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.749		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1452.00		NIST Webbook
rinpol	1450.00		NIST Webbook
ripol	1837.00		NIST Webbook
ripol	1831.00		NIST Webbook
tb	618.48	K	Joback Method
tc	847.90	K	Joback Method
tf	373.71	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.43	J/mol×K	618.48	Joback Method
cpg	564.39	J/mol×K	656.72	Joback Method
cpg	583.21	J/mol×K	694.95	Joback Method
cpg	601.19	J/mol×K	733.19	Joback Method
cpg	618.60	J/mol×K	771.43	Joback Method

cpg	635.74	J/mol×K	809.66	Joback Method
cpg	652.90	J/mol×K	847.90	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=R232421&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume