9-epi-3,6,6,9-Bisepoxy-farnesa-1,7(14),10-triene

Other names: 9-epi-3,6;6,9-Bisepoxyfarnesa-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	1450.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1452.00		NIST Webbook
ripol	1842.00		NIST Webbook
ripol	1834.00		NIST Webbook
ripol	1834.00		NIST Webbook
ripol	1842.00		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

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=R232550&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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