7-epi-7,10,Epoxyfarnesa-1,5,11-trien-3-ol

Inchi: InChI=1S/C16H26O2/c1-6-15(4,17)10-7-8-11-16(5)12-9-14(18-16)13(2)3/h6,8,11,14,17H
InchiKey: CYBFOKSTAJYZDI-SWAHVZKGSA-N
Formula: C16H26O2
SMILES: C=CC(C)(O)CCC=CC1(C)CCC(C(=C)C)O1
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	134.44	kJ/mol	Joback Method
hf	-252.88	kJ/mol	Joback Method
hfus	26.89	kJ/mol	Joback Method
hvap	68.60	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.774		Crippen Method
mcvol	224.280	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1539.00		NIST Webbook
rinpol	1539.00		NIST Webbook
ripol	2135.00		NIST Webbook
tb	689.63	K	Joback Method
tc	888.88	K	Joback Method
tf	367.89	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.37	J/mol×K	689.63	Joback Method
cpg	667.69	J/mol×K	722.84	Joback Method
cpg	684.20	J/mol×K	756.05	Joback Method
cpg	700.02	J/mol×K	789.26	Joback Method
cpg	715.31	J/mol×K	822.46	Joback Method
cpg	730.21	J/mol×K	855.67	Joback Method
cpg	744.85	J/mol×K	888.88	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=R232545&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