

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

Inchi:

InChI=1S/C15H24O2/c1-6-14(4,16)9-7-10-15(5)11-8-13(17-15)12(2)3/h6-7,10,13,16H,1-

InchiKey:

FYNUDQSLPSFSMZ-HKELBZMOSA-N

Formula:

C15H24O2

SMILES:

C=CC(C)(O)CC=CC1(C)CCC(C(=C)C)O1

Mol. weight [g/mol]:

236.35

Physical Properties

Property code	Value	Unit	Source
gf	126.02	kJ/mol	Joback Method
hf	-232.24	kJ/mol	Joback Method
hfus	24.30	kJ/mol	Joback Method
hvap	66.37	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.383		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1531.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1527.00		NIST Webbook
ripol	2122.00		NIST Webbook
ripol	2122.00		NIST Webbook
ripol	2116.00		NIST Webbook
ripol	2116.00		NIST Webbook
tb	666.75	K	Joback Method
tc	868.35	K	Joback Method
tf	356.62	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.11	J/mol×K	666.75	Joback Method
cpg	613.03	J/mol×K	700.35	Joback Method
cpg	629.08	J/mol×K	733.95	Joback Method

cpg	644.41	J/mol×K	767.55	Joback Method
cpg	659.15	J/mol×K	801.15	Joback Method
cpg	673.45	J/mol×K	834.75	Joback Method
cpg	687.46	J/mol×K	868.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232530&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

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