

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

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

LJPFBTWRZZGKFP-UHFFFAOYSA-N

C15H24O2

C=CC(C)(O)CCC1OC(C=C(C)C)CC1=C

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	1600.00		NIST Webbook
rinpol	1601.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1601.00		NIST Webbook
ripol	2229.00		NIST Webbook
ripol	2255.00		NIST Webbook
ripol	2255.00		NIST Webbook
ripol	2229.00		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

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=R232461&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

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