

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

<b>Other names:</b>	3-epi-3,6,6,9-Bisepoxy-farnesa-1,7(14),10-triene
<b>Inchi:</b>	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
<b>InchiKey:</b>	WKVFNUBTMXSGNM-UHFFFAOYSA-N
<b>Formula:</b>	C15H22O2
<b>SMILES:</b>	C=CC1(C)CCC2(OC(C=C(C)C)CC2=C)O1
<b>Mol. weight [g/mol]:</b>	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	1458.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
ripol	1870.00		NIST Webbook
ripol	1877.00		NIST Webbook
ripol	1877.00		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/molxK	618.48	Joback Method
cpg	564.39	J/molxK	656.72	Joback Method
cpg	583.21	J/molxK	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

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R232456&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R232456&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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