

# 11-epi-6,10-Epoxybisabol-3-en-12-al

<b>Inchi:</b>	InChI=1S/C15H24O2/c1-10-4-6-13-11(2)5-7-14(12(3)9-16)17-15(13)8-10/h4,9,11-15H,5-
<b>InchiKey:</b>	NPSHXIOPYGVQEX-SHIHICALSA-N
<b>Formula:</b>	C15H24O2
<b>SMILES:</b>	CC1=CCC2C(C)CCC(C(C)C=O)OC2C1
<b>Mol. weight [g/mol]:</b>	236.35

## Physical Properties

Property code	Value	Unit	Source
gf	-46.75	kJ/mol	Joback Method
hf	-455.36	kJ/mol	Joback Method
hfus	30.10	kJ/mol	Joback Method
hvap	60.85	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.361		Crippen Method
mvol	203.630	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1648.00		NIST Webbook
rinpol	1648.00		NIST Webbook
tb	647.40	K	Joback Method
tc	867.03	K	Joback Method
tf	335.46	K	Joback Method
vc	0.765	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.44	J/molxK	647.40	Joback Method
cpg	689.69	J/molxK	830.42	Joback Method
cpg	672.93	J/molxK	793.82	Joback Method
cpg	654.86	J/molxK	757.21	Joback Method
cpg	635.44	J/molxK	720.61	Joback Method
cpg	614.65	J/molxK	684.00	Joback Method
cpg	705.18	J/molxK	867.03	Joback Method
dvisc	0.0003630	Paxs	647.40	Joback Method

dvisc	0.0004488	Paxs	595.41	Joback Method
dvisc	0.0005779	Paxs	543.42	Joback Method
dvisc	0.0007849	Paxs	491.43	Joback Method
dvisc	0.0011462	Paxs	439.44	Joback Method
dvisc	0.0018530	Paxs	387.45	Joback Method
dvisc	0.0034763	Paxs	335.46	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=R233528&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R233528&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>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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