

# 1,5-Epoxy-nor-ketoguaiene

<b>Inchi:</b>	InChI=1S/C14H18O2/c1-8(2)9-6-11-10-4-5-14(11,3)16-12(7-9)13(10)15/h12H,4-7H2,1-3H
<b>InchiKey:</b>	ARIDDJHZLBMHHP-PYMCNQPYSA-N
<b>Formula:</b>	C14H18O2
<b>SMILES:</b>	CC(C)=C1CC2=C3CCC2(C)OC(C1)C3=O
<b>Mol. weight [g/mol]:</b>	218.29

## Physical Properties

Property code	Value	Unit	Source
gf	66.17	kJ/mol	Joback Method
hf	-259.25	kJ/mol	Joback Method
hfus	21.80	kJ/mol	Joback Method
hvap	57.24	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.934		Crippen Method
mcvol	174.380	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1614.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1619.00		NIST Webbook
tb	663.80	K	Joback Method
tc	906.68	K	Joback Method
tf	439.45	K	Joback Method
vc	0.671	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.12	J/molxK	663.80	Joback Method
cpg	515.10	J/molxK	704.28	Joback Method
cpg	532.15	J/molxK	744.76	Joback Method
cpg	548.47	J/molxK	785.24	Joback Method
cpg	564.30	J/molxK	825.72	Joback Method
cpg	579.85	J/molxK	866.20	Joback Method

## Sources

<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=R612921&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R612921&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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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