

# 14-Hydroxy-9-epi-(E)-caryophyllene oxide

<b>Inchi:</b>	InChI=1S/C15H24O2/c1-10-4-5-13-15(3,17-13)7-6-12-11(10)8-14(12,2)9-16/h11-13,16H
<b>InchiKey:</b>	XLKXIWMHACWINL-RDPXLKGRSA-N
<b>Formula:</b>	C15H24O2
<b>SMILES:</b>	<chem>C=C1CCC2OC2(C)CCC2C1CC2(C)CO</chem>
<b>Mol. weight [g/mol]:</b>	236.35

## Physical Properties

Property code	Value	Unit	Source
gf	25.11	kJ/mol	Joback Method
hf	-363.20	kJ/mol	Joback Method
hfus	23.17	kJ/mol	Joback Method
hvap	67.67	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.909		Crippen Method
mvol	197.070	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1669.00		NIST Webbook
rinpol	1667.00		NIST Webbook
tb	685.06	K	Joback Method
tc	897.27	K	Joback Method
tf	442.46	K	Joback Method
vc	0.741	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.01	J/mol×K	685.06	Joback Method
cpg	628.78	J/mol×K	720.43	Joback Method
cpg	646.86	J/mol×K	755.80	Joback Method
cpg	664.48	J/mol×K	791.17	Joback Method
cpg	681.90	J/mol×K	826.54	Joback Method
cpg	699.33	J/mol×K	861.90	Joback Method
cpg	717.01	J/mol×K	897.27	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=R610816&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R610816&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>rinpola:</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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