

# 7,11-Epoxy-eremophila-1,9-dien-8-«alpha»-ol

<b>Inchi:</b>	InChI=1S/C15H22O2/c1-10-6-5-7-11-8-12(16)15(9-14(10,11)4)13(2,3)17-15/h5,7-8,10,12
<b>InchiKey:</b>	IFTKMYUGODMWJL-BTQDYEIMSA-N
<b>Formula:</b>	C15H22O2
<b>SMILES:</b>	CC1CC=CC2=CC(O)C3(CC21C)OC3(C)C
<b>Mol. weight [g/mol]:</b>	234.33

## Physical Properties

Property code	Value	Unit	Source
gf	16.83	kJ/mol	Joback Method
hf	-328.11	kJ/mol	Joback Method
hfus	20.08	kJ/mol	Joback Method
hvap	67.60	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.827		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinsol	1726.00		NIST Webbook
tb	689.44	K	Joback Method
tc	911.79	K	Joback Method
tf	466.72	K	Joback Method
vc	0.727	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.67	J/mol×K	689.44	Joback Method
cpg	600.40	J/mol×K	726.50	Joback Method
cpg	617.81	J/mol×K	763.56	Joback Method
cpg	635.28	J/mol×K	800.61	Joback Method
cpg	653.17	J/mol×K	837.67	Joback Method
cpg	671.83	J/mol×K	874.73	Joback Method
cpg	691.65	J/mol×K	911.79	Joback Method

# Sources

<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=R198846&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R198846&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>
<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>

# 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>h vap:</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>m cvol:</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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