

# Eremophyla-9,11-dien-8-one

<b>Inchi:</b>	InChI=1S/C15H22O/c1-10(2)13-9-15(4)11(3)6-5-7-12(15)8-14(13)16/h8,11,13H,1,5-7,9H
<b>InchiKey:</b>	DIZRSLUNVNGBPA-ZLDLUXBVSA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	<chem>C=C(C)C1CC2(C)C(=CC1=O)CCCC2C</chem>
<b>Mol. weight [g/mol]:</b>	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	112.35	kJ/mol	Joback Method
hf	-212.82	kJ/mol	Joback Method
hfus	15.00	kJ/mol	Joback Method
hvap	52.65	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mvol	193.460	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
tb	637.25	K	Joback Method
tc	875.13	K	Joback Method
tf	366.05	K	Joback Method
vc	0.730	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.13	J/mol×K	637.25	Joback Method
cpg	562.46	J/mol×K	676.90	Joback Method
cpg	583.51	J/mol×K	716.54	Joback Method
cpg	603.42	J/mol×K	756.19	Joback Method
cpg	622.34	J/mol×K	795.83	Joback Method
cpg	640.42	J/mol×K	835.48	Joback Method
cpg	657.81	J/mol×K	875.13	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=R324877&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R324877&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>

# 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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