

# 1,2-Dehydrosesquicineole

<b>Inchi:</b>	InChI=1S/C15H24O/c1-12(2)6-5-9-15(4)13-7-10-14(3,16-15)11-8-13/h6-7H,5,8-11H2,1-4
<b>InchiKey:</b>	GWHXPRLXLILZQF-GICMACPYSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	CC(C)=CCCC1(C)OC2(C)CC=C1CC2
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	167.62	kJ/mol	Joback Method
hf	-167.43	kJ/mol	Joback Method
hfus	21.78	kJ/mol	Joback Method
hvap	52.35	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.391		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpole	1460.00		NIST Webbook
ripole	1738.00		NIST Webbook
ripole	1738.00		NIST Webbook
tb	600.23	K	Joback Method
tc	821.16	K	Joback Method
tf	356.26	K	Joback Method
vc	0.757	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.26	J/molxK	600.23	Joback Method
cpg	550.02	J/molxK	637.05	Joback Method
cpg	568.60	J/molxK	673.87	Joback Method
cpg	586.27	J/molxK	710.69	Joback Method
cpg	603.31	J/molxK	747.51	Joback Method
cpg	620.01	J/molxK	784.34	Joback Method
cpg	636.62	J/molxK	821.16	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=R232392&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R232392&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	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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