

# Caryophyllen-5-ol III

<b>Inchi:</b>	InChI=1S/C15H24O/c1-10-6-8-14(16)11(2)5-7-13-12(10)9-15(13,3)4/h5,12-14,16H,1,6-9
<b>InchiKey:</b>	DWUYGFWOANEJRE-BZMNMHEJSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	<chem>C=C1CCC(O)C(C)=CCC2C1CC2(C)C</chem>
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	52.10	kJ/mol	Joback Method
hf	-285.25	kJ/mol	Joback Method
hfus	19.98	kJ/mol	Joback Method
hvap	65.69	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
ripol	1642.00		NIST Webbook
ripol	2317.00		NIST Webbook
ripol	2317.00		NIST Webbook
tb	663.81	K	Joback Method
tc	872.81	K	Joback Method
tf	380.29	K	Joback Method
vc	0.735	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.12	J/molxK	663.81	Joback Method
cpg	595.62	J/molxK	698.64	Joback Method
cpg	614.14	J/molxK	733.48	Joback Method
cpg	631.79	J/molxK	768.31	Joback Method
cpg	648.66	J/molxK	803.14	Joback Method
cpg	664.87	J/molxK	837.98	Joback Method
cpg	680.52	J/molxK	872.81	Joback Method

# Sources

<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>
<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=R545747&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R545747&amp;Units=SI</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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