

# Caryophylla-3,8(15)-dien-5«alpha»-ol

<b>Inchi:</b>	InChI=1S/C15H26O/c1-12-7-8-14(16)13(2)6-5-10-15(3,4)11-9-12/h6,14,16H,1,5,7-11H2,
<b>InchiKey:</b>	PAGSXLWQSGUSAH-CNTYAIEFGSA-N
<b>Formula:</b>	C15H26O
<b>SMILES:</b>	C=C1CCC(O)C(C)=CCCC(C)(C)CC1
<b>Mol. weight [g/mol]:</b>	222.37

## Physical Properties

Property code	Value	Unit	Source
gf	-37.24	kJ/mol	Joback Method
hf	-356.19	kJ/mol	Joback Method
hfus	14.48	kJ/mol	Joback Method
hvap	66.61	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.230		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1643.00		NIST Webbook
rinpol	1652.00		NIST Webbook
ripol	2351.00		NIST Webbook
ripol	2351.00		NIST Webbook
tb	674.55	K	Joback Method
tc	889.40	K	Joback Method
tf	356.03	K	Joback Method
vc	0.754	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.82	J/molxK	674.55	Joback Method
cpg	617.83	J/molxK	710.36	Joback Method
cpg	637.75	J/molxK	746.17	Joback Method
cpg	656.63	J/molxK	781.97	Joback Method
cpg	674.56	J/molxK	817.78	Joback Method
cpg	691.61	J/molxK	853.59	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=R227182&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R227182&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>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>rinpol:</b>	Non-polar retention indices
<b>ripol:</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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