

# Caryophylla-2(12),6-dien-5 «alpha»-ol (=Caryophylladienol I)

**Inchi:** InChI=1S/C15H24O/c1-10-6-8-14(16)11(2)5-7-13-12(10)9-15(13,3)4/h5,13-14,16H,6-9H2  
**InchiKey:** AHWWWENJXIHBBP-KGYHHKMSA-N  
**Formula:** C15H24O  
**SMILES:** CC1=CCC2C(=C(C)CCC1O)CC2(C)C  
**Mol. weight [g/mol]:** 220.35

## Physical Properties

Property code	Value	Unit	Source
gf	17.43	kJ/mol	Joback Method
hf	-314.31	kJ/mol	Joback Method
hfus	20.51	kJ/mol	Joback Method
hvap	67.46	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.840		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
tb	678.44	K	Joback Method
tc	889.36	K	Joback Method
tf	396.65	K	Joback Method
vc	0.738	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.76	J/molxK	678.44	Joback Method
cpg	593.47	J/molxK	713.59	Joback Method
cpg	611.28	J/molxK	748.75	Joback Method
cpg	628.31	J/molxK	783.90	Joback Method
cpg	644.67	J/molxK	819.05	Joback Method
cpg	660.47	J/molxK	854.20	Joback Method
cpg	675.83	J/molxK	889.36	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R438114&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R438114&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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