

# Caryophylla-3(15),7(14)-dien-6«alpha»-ol

<b>Inchi:</b>	InChI=1S/C15H24O/c1-10-5-7-13-12(9-15(13,3)4)11(2)14(16)8-6-10/h12-14,16H,1-2,5-9
<b>InchiKey:</b>	SYKFIZVLWNPGLS-JXQTWKCFSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	C=C1CCC(O)C(=C)C2CC(C)(C)C2CC1
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	84.85	kJ/mol	Joback Method
hf	-247.32	kJ/mol	Joback Method
hfus	17.99	kJ/mol	Joback Method
hvap	64.90	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1636.00		NIST Webbook
tb	658.83	K	Joback Method
tc	866.81	K	Joback Method
tf	380.69	K	Joback Method
vc	0.733	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.21	J/mol×K	658.83	Joback Method
cpg	594.89	J/mol×K	693.49	Joback Method
cpg	613.57	J/mol×K	728.16	Joback Method
cpg	631.35	J/mol×K	762.82	Joback Method
cpg	648.34	J/mol×K	797.48	Joback Method
cpg	664.64	J/mol×K	832.14	Joback Method
cpg	680.34	J/mol×K	866.81	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R233791&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R233791&amp;Units=SI</a>
<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>

# 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>rinpol:</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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