

# 14-Hydroxy-4,5-dihydro-«beta»-caryophyllene

<b>Inchi:</b>	InChI=1S/C15H26O/c1-11-5-4-6-12(10-16)7-8-14-13(11)9-15(14,2)3/h12-14,16H,1,4-10H
<b>InchiKey:</b>	QPKKKWDNDWSIRV-UHFFFAOYSA-N
<b>Formula:</b>	C15H26O
<b>SMILES:</b>	<chem>C=C1CCCC(CO)CCC2C1CC2(C)C</chem>
<b>Mol. weight [g/mol]:</b>	222.37

## Physical Properties

Property code	Value	Unit	Source
gf	31.77	kJ/mol	Joback Method
hf	-331.56	kJ/mol	Joback Method
hfus	19.15	kJ/mol	Joback Method
hvap	64.74	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.778		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
ripol	2415.00		NIST Webbook
ripol	2415.00		NIST Webbook
ripol	2415.00		NIST Webbook
tb	659.67	K	Joback Method
tc	866.13	K	Joback Method
tf	367.01	K	Joback Method
vc	0.749	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.07	J/mol×K	659.67	Joback Method
cpg	619.70	J/mol×K	694.08	Joback Method
cpg	639.27	J/mol×K	728.49	Joback Method
cpg	657.89	J/mol×K	762.90	Joback Method
cpg	675.66	J/mol×K	797.31	Joback Method
cpg	692.70	J/mol×K	831.72	Joback Method
cpg	709.11	J/mol×K	866.13	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=R336157&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R336157&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>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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