

# 12-Hydroxy-«beta»-caryophyllene acetate

<b>Inchi:</b>	InChI=1S/C17H26O2/c1-12-6-5-7-13(2)15-10-17(4,11-19-14(3)18)16(15)9-8-12/h6,15-16
<b>InchiKey:</b>	VKTLOEXWZVKMMV-LAPICBTHSA-N
<b>Formula:</b>	C17H26O2
<b>SMILES:</b>	<chem>C=C1CCC=C(C)CCC2C1CC2(C)COC(C)=O</chem>
<b>Mol. weight [g/mol]:</b>	262.39

## Physical Properties

Property code	Value	Unit	Source
gf	-20.45	kJ/mol	Joback Method
hf	-398.76	kJ/mol	Joback Method
hfus	22.79	kJ/mol	Joback Method
hvap	62.93	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.268		Crippen Method
mcvol	227.510	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
ripol	2331.00		NIST Webbook
ripol	2331.00		NIST Webbook
ripol	2331.00		NIST Webbook
tb	698.35	K	Joback Method
tc	919.73	K	Joback Method
tf	418.41	K	Joback Method
vc	0.853	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.66	J/molxK	698.35	Joback Method
cpg	691.18	J/molxK	735.25	Joback Method
cpg	711.58	J/molxK	772.14	Joback Method
cpg	730.98	J/molxK	809.04	Joback Method
cpg	749.50	J/molxK	845.93	Joback Method
cpg	767.26	J/molxK	882.83	Joback Method
cpg	784.38	J/molxK	919.73	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R418229&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R418229&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>hvp:</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>ripl:</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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