

# (6R)-Hydroxy-«beta»-caryophyllene acetate

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

## Physical Properties

Property code	Value	Unit	Source
gf	-28.16	kJ/mol	Joback Method
hf	-419.10	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	62.62	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.267		Crippen Method
mvol	227.510	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	1771.00		NIST Webbook
tb	693.68	K	Joback Method
tc	915.09	K	Joback Method
tf	414.17	K	Joback Method
vc	0.852	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.67	J/mol×K	693.68	Joback Method
cpg	693.69	J/mol×K	730.58	Joback Method
cpg	714.56	J/mol×K	767.48	Joback Method
cpg	734.39	J/mol×K	804.38	Joback Method
cpg	753.29	J/mol×K	841.28	Joback Method
cpg	771.37	J/mol×K	878.19	Joback Method
cpg	788.75	J/mol×K	915.09	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R619006&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R619006&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>h vap:</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>m cvol:</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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