

# 4-Acetoxy-germacra-1,8(11)dien-9-one

<b>Inchi:</b>	InChI=1S/C17H26O3/c1-11(2)15-8-7-13(4)17(20-14(5)18)9-6-12(3)10-16(15)19/h6,13,17
<b>InchiKey:</b>	JCXJNMDQQLRIGL-WUXMJOGZSA-N
<b>Formula:</b>	C17H26O3
<b>SMILES:</b>	CC(=O)OC1CC=C(C)CC(=O)C=C(C(C)C)CCC1C
<b>Mol. weight [g/mol]:</b>	278.39

## Physical Properties

Property code	Value	Unit	Source
gf	-238.67	kJ/mol	Joback Method
hf	-654.82	kJ/mol	Joback Method
hfus	26.44	kJ/mol	Joback Method
hvap	69.47	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.980		Crippen Method
mcvol	239.940	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinsol	1875.00		NIST Webbook
tb	775.09	K	Joback Method
tc	1006.36	K	Joback Method
tf	420.47	K	Joback Method
vc	0.888	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.09	J/mol×K	775.09	Joback Method
cpg	758.07	J/mol×K	813.63	Joback Method
cpg	777.25	J/mol×K	852.18	Joback Method
cpg	794.59	J/mol×K	890.72	Joback Method
cpg	810.03	J/mol×K	929.27	Joback Method
cpg	823.53	J/mol×K	967.81	Joback Method
cpg	835.04	J/mol×K	1006.36	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R547921&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R547921&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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