

# Acetic acid, (17beta-hydroxy-3-oxo-5beta-androstan-16-beta-y lactone

InChI: InChI=1S/C21H30O3/c1-20-7-5-14(22)11-13(20)3-4-15-16(20)6-8-21(2)17(15)9-12-10-18  
InChIKey: QLIYDRBKFUETLS-UHFFFAOYSA-N  
Formula: C21H30O3  
SMILES: CC12CCC(=O)CC1CCC1C2CCC2(C)C1CC1CC(=O)OC12  
Mol. weight [g/mol]: 330.46  
CAS: 104713-06-6

## Physical Properties

Property code	Value	Unit	Source
gf	3.78	kJ/mol	Joback Method
hf	-581.51	kJ/mol	Joback Method
hfus	27.94	kJ/mol	Joback Method
hvap	72.54	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.140		Crippen Method
mcvol	261.460	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
tb	883.99	K	Joback Method
tc	1147.88	K	Joback Method
tf	596.62	K	Joback Method
vc	0.985	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.32	J/molxK	883.99	Joback Method
cpg	1013.92	J/molxK	927.97	Joback Method
cpg	1043.59	J/molxK	971.95	Joback Method
cpg	1073.76	J/molxK	1015.93	Joback Method
cpg	1104.87	J/molxK	1059.92	Joback Method
cpg	1137.36	J/molxK	1103.90	Joback Method
cpg	1171.67	J/molxK	1147.88	Joback Method

# Sources

<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=C104713066&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C104713066&amp;Units=SI</a>
<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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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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