

# 5Beta-androstan-16beta-ylacetic acid lactone, 3beta,17beta-dihydroxy-

<b>Inchi:</b>	InChI=1S/C21H32O3/c1-20-7-5-14(22)11-13(20)3-4-15-16(20)6-8-21(2)17(15)9-12-10-18
<b>InchiKey:</b>	TWLWASBVSWBNCK-WVUNLQOWSA-N
<b>Formula:</b>	C21H32O3
<b>SMILES:</b>	CC12CCC(O)CC1CCC1C2CCC2(C)C1CC1CC(=O)OC12
<b>Mol. weight [g/mol]:</b>	332.48
<b>CAS:</b>	96191-75-2

## Physical Properties

Property code	Value	Unit	Source
gf	-18.16	kJ/mol	Joback Method
hf	-616.38	kJ/mol	Joback Method
hfus	33.59	kJ/mol	Joback Method
hvap	84.66	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.932		Crippen Method
mcvol	265.760	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
tb	903.68	K	Joback Method
tc	1141.33	K	Joback Method
tf	584.98	K	Joback Method
vc	0.996	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1022.23	J/molxK	903.68	Joback Method
cpg	1049.39	J/molxK	943.29	Joback Method
cpg	1076.88	J/molxK	982.90	Joback Method
cpg	1105.05	J/molxK	1022.50	Joback Method
cpg	1134.27	J/molxK	1062.11	Joback Method
cpg	1164.88	J/molxK	1101.72	Joback Method
cpg	1197.24	J/molxK	1141.33	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=C96191752&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C96191752&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>mccvol:</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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