

# 3Beta-acetoxy-17beta-hydroxy-5alpha-androstan- acid lactone

InChI: InChI=1S/C23H34O4/c1-13(24)26-16-6-8-22(2)15(12-16)4-5-17-18(22)7-9-23(3)19(17)10  
InChIKey: PAONJAURFWGCAT-UHFFFAOYSA-N

Formula: C23H34O4

SMILES: CC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C3CC3CC(=O)OC32)C1

Mol. weight [g/mol]: 374.51

CAS: 125567-32-0

## Physical Properties

Property code	Value	Unit	Source
gf	-98.42	kJ/mol	Joback Method
hf	-750.23	kJ/mol	Joback Method
hfus	37.46	kJ/mol	Joback Method
hvap	81.59	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.502		Crippen Method
mcvol	295.510	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
tb	933.55	K	Joback Method
tc	1181.55	K	Joback Method
tf	618.86	K	Joback Method
vc	1.113	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.12	J/molxK	933.55	Joback Method
cpg	1162.79	J/molxK	974.88	Joback Method
cpg	1192.81	J/molxK	1016.22	Joback Method
cpg	1223.56	J/molxK	1057.55	Joback Method
cpg	1255.42	J/molxK	1098.88	Joback Method
cpg	1288.78	J/molxK	1140.22	Joback Method
cpg	1324.02	J/molxK	1181.55	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.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=C125567320&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C125567320&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>hvac:</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>mccol:</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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