

# 5-Androstene-3beta,17beta-diol,16beta-ylacetic acid, 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: UHRRKAOLVBHHLU-UHFFFAOYSA-N

Formula: C21H30O3

SMILES: CC12CCC(O)CC1=CCC1C2CCC2(C)C1CC1CC(=O)OC12

Mol. weight [g/mol]: 330.46

CAS: 10458-98-7

## Physical Properties

Property code	Value	Unit	Source
gf	9.88	kJ/mol	Joback Method
hf	-549.73	kJ/mol	Joback Method
hfus	33.35	kJ/mol	Joback Method
hvap	85.93	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	3.852		Crippen Method
mcvol	261.460	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
tb	912.49	K	Joback Method
tc	1152.32	K	Joback Method
tf	602.50	K	Joback Method
vc	0.983	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.17	J/molxK	912.49	Joback Method
cpg	1015.67	J/molxK	952.46	Joback Method
cpg	1042.72	J/molxK	992.43	Joback Method
cpg	1070.72	J/molxK	1032.40	Joback Method
cpg	1100.01	J/molxK	1072.37	Joback Method
cpg	1130.98	J/molxK	1112.35	Joback Method
cpg	1163.99	J/molxK	1152.32	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C10458987&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10458987&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>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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