

# Androstane-17beta-carboxylic acid,5alpha,6beta-dichloro-3-hydroxy-, acetate

InChI: InChI=1S/C22H32Cl2O4/c1-12(25)28-13-6-9-21(3)16-7-8-20(2)15(4-5-17(20)19(26)27)14  
InChIKey: QQUMOUYAMOTHCF-UHFFFAOYSA-N

Formula: C22H32Cl2O4

SMILES: CC(=O)OC1CCC2(C)C3CCC4(C)C(C(=O)O)CCC4C3CC(Cl)C2(Cl)C1

Mol. weight [g/mol]: 431.39

CAS: 116405-12-0

## Physical Properties

Property code	Value	Unit	Source
gf	-261.68	kJ/mol	Joback Method
hf	-834.08	kJ/mol	Joback Method
hfus	38.10	kJ/mol	Joback Method
hvap	101.43	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.240		Crippen Method
mcvol	316.760	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
tb	1025.64	K	Joback Method
tc	1267.28	K	Joback Method
tf	685.11	K	Joback Method
vc	1.192	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.33	J/molxK	1025.64	Joback Method
cpg	1225.28	J/molxK	1065.91	Joback Method
cpg	1262.79	J/molxK	1106.19	Joback Method
cpg	1303.34	J/molxK	1146.46	Joback Method
cpg	1347.41	J/molxK	1186.73	Joback Method
cpg	1395.46	J/molxK	1227.01	Joback Method
cpg	1447.97	J/molxK	1267.28	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=C116405120&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116405120&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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