

# 4-Chloro-17alpha-methyl-19-nortestosterone

<b>Inchi:</b>	InChI=1S/C19H27ClO2/c1-18-9-7-12-11-5-6-16(21)17(20)14(11)4-3-13(12)15(18)8-10-19
<b>InchiKey:</b>	KLBQJNJDOQGAFJ-UHFFFAOYSA-N
<b>Formula:</b>	C19H27ClO2
<b>SMILES:</b>	CC1(O)CCC2C3CCC4=C(Cl)C(=O)CCC4C3CCC21C
<b>Mol. weight [g/mol]:</b>	322.87
<b>CAS:</b>	3415-90-5

## Physical Properties

Property code	Value	Unit	Source
gf	4.56	kJ/mol	Joback Method
hf	-456.12	kJ/mol	Joback Method
hfus	24.79	kJ/mol	Joback Method
hvap	82.41	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.446		Crippen Method
mcvol	250.510	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
tb	880.12	K	Joback Method
tc	1119.74	K	Joback Method
tf	582.13	K	Joback Method
vc	0.943	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.10	J/molxK	880.12	Joback Method
cpg	894.96	J/molxK	920.06	Joback Method
cpg	919.16	J/molxK	959.99	Joback Method
cpg	944.02	J/molxK	999.93	Joback Method
cpg	969.90	J/molxK	1039.86	Joback Method
cpg	997.10	J/molxK	1079.80	Joback Method
cpg	1025.96	J/molxK	1119.74	Joback Method

# Sources

<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=C3415905&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3415905&amp;Units=SI</a>
<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>

# 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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