

# 19-Nortestosterone, 4-chloro-, p-chlorophenoxyacetic acid ester

<b>Inchi:</b>	InChI=1S/C26H30Cl2O4/c1-26-13-12-18-17-8-10-22(29)25(28)20(17)7-6-19(18)21(26)9-
<b>InchiKey:</b>	RIFKMUCBGBCCAA-UHFFFAOYSA-N
<b>Formula:</b>	C26H30Cl2O4
<b>SMILES:</b>	CC12CCC3C4CCC(=O)C(Cl)=C4CCC3C1CCC2OC(=O)COc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	477.42
<b>CAS:</b>	22467-98-7

## Physical Properties

Property code	Value	Unit	Source
gf	-42.26	kJ/mol	Joback Method
hf	-631.31	kJ/mol	Joback Method
hfus	46.95	kJ/mol	Joback Method
hvap	101.35	kJ/mol	Joback Method
log10ws	-7.36		Crippen Method
logp	6.339		Crippen Method
mvol	345.060	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
tb	1115.66	K	Joback Method
tc	1380.59	K	Joback Method
tf	739.55	K	Joback Method
vc	1.300	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1254.56	J/molxK	1115.66	Joback Method
cpg	1277.74	J/molxK	1159.82	Joback Method
cpg	1300.95	J/molxK	1203.97	Joback Method
cpg	1324.45	J/molxK	1248.13	Joback Method
cpg	1348.52	J/molxK	1292.28	Joback Method
cpg	1373.43	J/molxK	1336.44	Joback Method
cpg	1399.46	J/molxK	1380.59	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=C22467987&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22467987&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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