

19-Nortestosterone, 4-chloro-, acetate

Other names:	4-chloro-17«beta»-hydroxyestr-4-en-3-one 17-acetate
Inchi:	InChI=1S/C20H27ClO3/c1-11(22)24-18-8-6-16-14-3-4-15-12(5-7-17(23)19(15)21)13(14)
InchiKey:	FNMAFGQVNCRKGS-UHFFFAOYSA-N
Formula:	C20H27ClO3
SMILES:	CC(=O)OC1CCC2C3CCC4=C(Cl)C(=O)CCC4C3CCC12C
Mol. weight [g/mol]:	350.88
CAS:	1164-99-4

Physical Properties

Property code	Value	Unit	Source
gf	-78.63	kJ/mol	Joback Method
hf	-584.57	kJ/mol	Joback Method
hfus	32.38	kJ/mol	Joback Method
hvap	78.26	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.626		Crippen Method
mcvol	266.170	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
tb	886.87	K	Joback Method
tc	1134.23	K	Joback Method
tf	580.84	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	917.22	J/molxK	886.87	Joback Method
cpg	939.72	J/molxK	928.10	Joback Method
cpg	961.43	J/molxK	969.32	Joback Method
cpg	982.54	J/molxK	1010.55	Joback Method
cpg	1003.28	J/molxK	1051.78	Joback Method
cpg	1023.85	J/molxK	1093.01	Joback Method
cpg	1044.47	J/molxK	1134.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1164994&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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