

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

Inchi:	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
InchiKey:	KLBQJNJDOQGAFJ-UHFFFAOYSA-N
Formula:	C19H27ClO2
SMILES:	CC1(O)CCC2C3CCC4=C(Cl)C(=O)CCC4C3CCC21C
Mol. weight [g/mol]:	322.87
CAS:	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

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=C3415905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	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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