Androsterone

Other names:	3-Epihydroxyetioallocholan-17-one
	3-«alpha»-Hydroxy-5-«alpha»-androstan-17-one
	3-Â«alphaÂ»-Hydroxy-5-Â«alphaÂ»-androstan-17-one
	3«alpha»-Hydroxy-17-androstanone
	3«alpha»-Hydroxyetioallocholan-17-one
	3Â«alphaÂ»-Hydroxy-17-androstanone
	3Â«alphaÂ»-Hydroxyetioallocholan-17-one
	5-«alpha»-Androstan-3-«alpha»-ol-17-one
	5-Â«alphaÂ»-Androstan-3-Â«alphaÂ»-ol-17-one
	5«alpha»-Androstan-17-one, 3«alpha»-hydroxy-
	5«alpha»-Androstane-3«alpha»-ol-17-one
	5«alpha»-Androsterone
	5Â«alphaÂ»-Androstan-17-one, 3Â«alphaÂ»-hydroxy-
	5Â«alphaÂ»-Androstane-3Â«alphaÂ»-ol-17-one
	5Â«alphaÂ»-Androsterone
	Androkinine
	Androstan-17-one, 3-hydroxy-, (3«alpha»,5«alpha»)-
	Androstan-17-one, 3-hydroxy-, (3Â«alphaÂ»,5Â«alphaÂ»)-
	Androstanon-3-«alpha»-ol-17-one
	Androstanon-3-Â«alphaÂ»-ol-17-one
	Androtine
	Atromide ICI
	NSC 9898
	U 6036
	cis-Androsterone
Inchi:	InChI=1S/C19H30O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14
InchiKey:	QGXBDMJGAMFCBF-WRBSTAHLSA-N
Formula:	C19H30O2
SMILES:	CC12CCC3C(CCC4CC(O)CCC43C)C1CCC2=O
Mol. weight [g/mol]:	290.44
CAS:	53-41-8

Physical Properties

Property code	Value	Unit	Source
chs	-11090.00 ± 30.00	kJ/mol	NIST Webbook
gf	-1.92	kJ/mol	Joback Method

hf	-495.56	kJ/mol	Joback Method
hfus	21.22	kJ/mol	Joback Method
hvap	76.10	kJ/mol	Joback Method
log10ws	-4.40		Estimated Solubility Method
log10ws	-4.16		Aqueous Solubility Prediction Method
logp	3.959		Crippen Method
mcvol	242.570	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2484.00		NIST Webbook
rinpol	2488.00		NIST Webbook
rinpol	2488.00		NIST Webbook
rinpol	2480.00		NIST Webbook
rinpol	2498.00		NIST Webbook
rinpol	2480.00		NIST Webbook
rinpol	2484.00		NIST Webbook
rinpol	2486.00		NIST Webbook
tb	828.90	K	Joback Method
tc	1062.98	K	Joback Method
tf	522.17	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.61	J/mol×K	828.90	Joback Method
cpg	895.49	J/mol×K	867.91	Joback Method
cpg	920.14	J/mol×K	906.93	Joback Method
cpg	944.87	J/mol×K	945.94	Joback Method
cpg	969.98	J/mol×K	984.95	Joback Method
cpg	995.80	J/mol×K	1023.97	Joback Method
cpg	1022.62	J/mol×K	1062.98	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53418&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume