Epiandrosterone

Other names:	3-Epiandrosterone
	3-«beta»Hydroxyandrostan-17-one
	3-Â«betaÂ»Hydroxyandrostan-17-one
	3Beta-hydroxy-5alpha-androstan-17-one
	3«beta»-Androsterone
	3«beta»-Hydroxy-5«alpha»-androstan-17-one
	3«beta»-Hydroxyetioallocholan-17-one
	3Â«betaÂ»-Androsterone
	3Â«betaÂ»-Hydroxy-5Â«alphaÂ»-androstan-17-one
	3Â«betaÂ»-Hydroxyetioallocholan-17-one
	5A-Androstan-3B-ol-17-one
	5«alpha»-Androstan-17-one, 3«beta»-hydroxy-
	5«alpha»-Androstan-3«beta»-ol-17-one
	5Â«alphaÂ»-Androstan-17-one, 3Â«betaÂ»-hydroxy-
	5Â«alphaÂ»-Androstan-3Â«betaÂ»-ol-17-one
	Androstan-17-one, 3-hydroxy-, (3«beta»,5«alpha»)-
	Androstan-17-one, 3-hydroxy-, (3Â«betaÂ»,5Â«alphaÂ»)-
	Androsterone, (3«beta»)-
	Androsterone, (3Â«betaÂ»)-
	Androsterone, epi-
	Androsterone, trans-
	D-Epiandrosterone
	NSC 93996
	iso-Androsterone
	trans-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-DPSNFPCPSA-N
Formula:	C19H30O2
SMILES:	CC12CCC3C(CCC4CC(O)CCC43C)C1CCC2=O
Mol. weight [g/mol]:	290.44
CAS:	481-29-8

Physical Properties

Property code	Value	Unit	Source
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	-4.16		Estimated Solubility Method
logp	3.959		Crippen Method
mcvol	242.570	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2504.00		NIST Webbook
rinpol	2504.00		NIST Webbook
rinpol	2482.00		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

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=C481298&Units=SI

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

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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume