Androstan-17-one, 3,11-dihydroxy-, (3«alpha»,5«beta»,11«beta»)-

Other names: 11-Hydroxyetiocholanolone
3«alpha»,11«beta»-Dihydroxy-5«beta»-androstan-17-one
3Â«alphaÂ»,11Â«betaÂ»-Dihydroxy-5Â«betaÂ»-androstan-17-one
5«beta»-Androstan-3«alpha»,11«beta»-diol-17-one
5Â«betaÂ»-Androstan-3Â«alphaÂ»,11Â«betaÂ»-diol-17-one
hydroxyisoandrosterone

Inchi: InChI=1S/C19H30O3/c1-18-8-7-12(20)9-11(18)3-4-13-14-5-6-16(22)19(14,2)10-15(21)17

InchiKey: PIXFHVWJOVNKQK-BEWPHQSDSA-N

Formula: C19H30O3

SMILES: CC12CC(O)C3C(CCC4CC(O)CCC43C)C1CCC2=O

Mol. weight [g/mol]: 306.44

CAS: 739-26-4

Physical Properties

Property code	Value	Unit	Source
gf	-146.45	kJ/mol	Joback Method
hf	-668.13	kJ/mol	Joback Method
hfus	26.38	kJ/mol	Joback Method
hvap	92.47	kJ/mol	Joback Method
log10ws	-3.59		Aqueous Solubility Prediction Method
logp	2.930		Crippen Method
mcvol	248.440	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
tb	916.41	K	Joback Method
tc	1140.77	K	Joback Method
tf	578.75	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.07	J/mol×K	916.41	Joback Method
cpg	975.05	J/mol×K	953.80	Joback Method

cpg	999.37	J/mol×K	991.20	Joback Method
cpg	1024.29	J/mol×K	1028.59	Joback Method
cpg	1050.08	J/mol×K	1065.98	Joback Method
cpg	1077.00	J/mol×K	1103.38	Joback Method
cpg	1105.34	J/mol×K	1140.77	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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C739264&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