Pregnenolone

Other names:	3-Hydroxypregn-5-en-20-one
	3-Hydroxypregn-5-en-20-one, (3«beta»)-
	3-Hydroxypregn-5-en-20-one, (3Â«betaÂ»)-
	3«beta»-Hydroxy-«DELTA»5-pregnen-20-one
	3«beta»-Hydroxypregn-5-en-20-one
	3Â«betaÂ»-Hydroxy-Â«DELTAÂ»5-pregnen-20-one
	3Â«betaÂ»-Hydroxypregn-5-en-20-one
	5-Pregnen-3«beta»-ol-20-one
	5-Pregnen-3Â«betaÂ»-ol-20-one
	5-Pregnenolone
	Arthenolone
	Bina-Skin
	Enelone
	NSC 1616
	Natolone
	Pregn-5-en-20-one, 3-hydroxy-, (3«beta»)-
	Pregn-5-en-20-one, 3-hydroxy-, (3Â«betaÂ»)-
	Pregn-5-en-20-one, 3«beta»-hydroxy-
	Pregn-5-en-20-one, 3Â«betaÂ»-hydroxy-
	Pregnetan
	Pregneton
	Pregnolon
	Pregnolone
	Prenolon
	Regnosone
	Skinostelon
	«DELTA»5-Pregnen-3«beta»-ol-20-one
	«DELTA»5-Pregnenolone
	Â«DELTAÂ»5-Pregnen-3Â«betaÂ»-ol-20-one
	Â«DELTAÂ»5-Pregnenolone
Inchi:	InChI=1S/C21H32O2/c1-13(22)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9-11-2
InchiKey:	ORNBQBCIOKFOEO-UOZQCWKMSA-N
Formula:	C21H32O2
SMILES:	CC(=O)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	316.48
CAS:	145-13-1

Physical Properties

Property code	Value	Unit	Source
gf	28.92	kJ/mol	Joback Method
hf	-465.41	kJ/mol	Joback Method
hfus	29.32	kJ/mol	Joback Method
hvap	84.00	kJ/mol	Joback Method
log10ws	-4.65		Aqueous Solubility Prediction Method
log10ws	-4.65		Estimated Solubility Method
logp	4.515		Crippen Method
mcvol	266.450	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	2775.20		NIST Webbook
rinpol	2775.20		NIST Webbook
tb	864.85	K	Joback Method
tc	1091.42	K	Joback Method
tf	539.70	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.54	J/mol×K	864.85	Joback Method
cpg	974.02	J/mol×K	902.61	Joback Method
cpg	998.64	J/mol×K	940.37	Joback Method
cpg	1023.72	J/mol×K	978.14	Joback Method
cpg	1049.57	J/mol×K	1015.90	Joback Method
cpg	1076.50	J/mol×K	1053.66	Joback Method
cpg	1104.85	J/mol×K	1091.42	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=C145131&Units=SI
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

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