3-Hydroxyestra-1,3,5(10)-trien-17-one

Other names:

(+)-Estrone
1,3,5(10)-Estratrien-3-ol-17-one
1,3,5(10)-Oestratrien-3-ol-17-one
1,3,5-Oestratrien-3-ol-17-one
3-Hydroxy-1,3,5(10)-oestratrien-17-one
3-Hydroxy-17-keto-estra-1,3,5-triene
3-Hydroxy-17-keto-oestra-1,3,5-triene
3-Hydroxy-oestra-1,3,5(10)-trien-17-one
3-Hydroxyestra-1,3,5(10)-triene-17-one
3-hydroxy-1,3,5(10)-estratrien-17-one
3-hydroxy-13-methyl-7,8,9,11,12,14,15,16-octahydro-6H-cyclopenta[a]phenanthren-17-or
Aquacrine
Crinovaryl
Cristallovar
Crystogen
Destrone
Disynformon
E(sub 1)
Endofolliculina
Esterone
Estra-1,3,5(10)-trien-17-one, 3-hydroxy-
Estrin
Estrol
Estron
Estrona
Estrone-A
Estrugenone
Estrusol
Fem-O-Gen
Femestrone inj.
Femestrone injection
Femidyn
Fermidyn
Folikrin
Folipex
Folisan
Follestrine
Follestrol
Follicular hormone
Folliculin

Folliculine
Folliculine benzoate
Folliculinum
Follicunodis
Follidrin
Follidrin (tablets)
Glandubolin
Hiestrone
Hormestrin
Hormofollin
Hormovarine
Kestrone
Ketodestrin
Ketohydroxy-Estratriene
Ketohydroxyestrin
Ketohydroxyoestrin
Kolpon
Menagen
Menformon
Menformon A
Mestronaq
Oestrin
Oestroform
Oestrone
Oestroperos
Ovifollin
Perlatan
Solliculin
Theelin
Thelestrin
Thelykinin
Thynestron
Tokokin
Unden
Unden (pharmaceutical)
WAY 164397
Wynestron
delta-1,3,5-Estratrien-3«beta»-ol-17-one
delta-1,3,5-Oestratrien-3«beta»-ol-17-one
estrone
estrovarin
«DELTA»-1,3,5(10)-Estratrien-3-ol-17-one

Inchi: InChI=1S/C18H22O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20

InchiKey: DNXHEGUUPJUMQT-UHFFFAOYSA-N
Formula: C18H22O2
SMILES: CC12CCC3c4ccc(O)cc4CCC3C1CCC2=O
Mol. weight [g/mol]: 270.37

Physical Properties

Property code	Value	Unit	Source
hfus	45.11	kJ/mol	Experimental solubility for betulin and estrone in various solvents within the temperature range T = (293.2 to 328.2) K
ie	8.02	eV	Cheméo Relay (1.0)
log10ws	-4.23		Aqueous Solubility Prediction Method
log10ws	-3.96		Estimated Solubility Method
log10ws	-3.96		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	3.817		Crippen Method
mcvol	215.580	ml/mol	McGowan Method
rinpol	2736.60		NIST Webbook
rinpol	2755.90		NIST Webbook
rinpol	2756.20		NIST Webbook
rinpol	2693.80		NIST Webbook
tf	457.25	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.07	J/mol×K	815.67	Joback Method
cpg	736.60	J/mol×K	859.68	Joback Method
cpg	757.77	J/mol×K	903.68	Joback Method
cpg	778.96	J/mol×K	947.69	Joback Method
cpg	800.56	J/mol×K	991.70	Joback Method
cpg	822.93	J/mol×K	1035.71	Joback Method
cpg	846.45	J/mol×K	1079.71	Joback Method

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
Cheméo Relay (1.0):	
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53167&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0, beta):	
Experimental solubility for betulin and estrone in various solvents within the temperature range T = (283.2 to 328.2) K:	https://www.doi.org/10.1016/j.jct.2016.02.006
Aqueous Solubilities of Estrone, 17β-Estradiol, 17α-Ethynylestradiol, and Bisphenol A:	https://www.doi.org/10.1021/je050318c

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point