

Estriol

Other names:

(16.alpha.,17.beta.)-estra-1,3,5(10)-triene-3,16,17-triol
(16«alpha»,17«beta»)-Estra-1,3,5(10)-triene-3,16,17-triol
(16«alpha»,17«beta»)-Oestra-1,3,5(10)-triene-3,16,17-triol
(16Â«alphaÂ»,17Â«betaÂ»)-Estra-1,3,5(10)-triene-3,16,17-triol
(16Â«alphaÂ»,17Â«betaÂ»)-Oestra-1,3,5(10)-triene-3,16,17-triol
(8R,9S,13S,14S,16R,17R)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cycloper
1,3,5(10)-Estratrien-3,16«alpha»,17«beta»-triol
1,3,5(10)-Estratrien-3,16Â«alphaÂ»,17Â«betaÂ»-triol
1,3,5(10)-Estratriene-3,16«alpha»,17«beta»-Triol
1,3,5(10)-Estratriene-3,16Â«alphaÂ»,17Â«betaÂ»-Triol
1,3,5-Estratriene-3«beta»,16-«alpha»,17-«beta»-triol
1,3,5-Estratriene-3Â«betaÂ»,16-Â«alphaÂ»,17-Â«betaÂ»-triol
1,3,5-Oestratriene-3-«beta»,16«alpha»,17«beta»-triol
1,3,5-Oestratriene-3-Â«betaÂ»,16Â«alphaÂ»,17Â«betaÂ»-triol
16«alpha»,17«beta»-Estriol
16«alpha»,17«beta»-Oestriol
16«alpha»-Estriol
16«alpha»-Hydroxy-17«beta»-estradiol
16«alpha»-Hydroxyestradiol
16«alpha»-Hydroxyoestradiol
16Â«alphaÂ»,17Â«betaÂ»-Estriol
16Â«alphaÂ»,17Â«betaÂ»-Oestriol
16Â«alphaÂ»-Estriol
16Â«alphaÂ»-Hydroxy-17Â«betaÂ»-estradiol
16Â«alphaÂ»-Hydroxyestradiol
16Â«alphaÂ»-Hydroxyoestradiol
3,16-«alpha»,17-«beta»-Oestriol
3,16-«alpha»,17-«beta»-Trihydroxyoestra-1,3,5(10)-triene
3,16-Â«alphaÂ»,17-Â«betaÂ»-Oestriol
3,16-Â«alphaÂ»,17-Â«betaÂ»-Trihydroxyoestra-1,3,5(10)-triene
3,16«alpha»,17«beta»-Estriol
3,16«alpha»,17«beta»-Trihydroxy-1,3,5(10)-estratriene
3,16«alpha»,17«beta»-Trihydroxy-«delta»-1,3,5-estratriene
3,16«alpha»,17«beta»-Trihydroxy-«delta»-1,3,5-oestratriene
3,16«alpha»,17«beta»-Trihydroxyestra-1,3,5(10)-triene
3,16Â«alphaÂ»,17Â«betaÂ»-Estriol
3,16Â«alphaÂ»,17Â«betaÂ»-Trihydroxy-1,3,5(10)-estratriene
3,16Â«alphaÂ»,17Â«betaÂ»-Trihydroxy-Â«deltaÂ»-1,3,5-estratriene
3,16Â«alphaÂ»,17Â«betaÂ»-Trihydroxy-Â«deltaÂ»-1,3,5-oestratriene
3,16Â«alphaÂ»,17Â«betaÂ»-Trihydroxyestra-1,3,5(10)-triene

A 13610
Aacifemine
Colpogyn
Colpovister
Destriol
Deuslon A
Estra-1(10),2,4-triene-3,16,17-triol
Estra-1,3,5(10)-trien-3,16«alpha»,17«beta»-triol
Estra-1,3,5(10)-trien-3,16«alpha»,17«beta»-triol
Estra-1,3,5(10)-triene-3,16,17-triol, (16«alpha»,17«beta»)-
Estra-1,3,5(10)-triene-3,16,17-triol, (16«alpha»,17«beta»)-
Estra-1,3,5(10)-triene-3,16-«alpha», 17-«beta»-triol
Estra-1,3,5(10)-triene-3,16-«alpha», 17-«beta»-triol
Estra-1,3,5(10)-triene-3,16«alpha»,17«beta»-triol
Estra-1,3,5(10)-triene-3,16«alpha»,17«beta»-triol
Estratriol
Estriel
Estriolo
Follicular hormone
Follicular hormone hydrate
Gynaesan
Gynasan
Hemostyptanon
Holin
Hormomed
Hormonin
Incurin
Klimax E
Klimoral
NSC-12169
OE3
Oekolp
Oestra-1,3,5(10)-triene-3,16«alpha», 17«beta»-triol
Oestra-1,3,5(10)-triene-3,16«alpha», 17«beta»-triol
Oestratriol
Oestriol
Orestin
Orgastypin
Ortho-Gynest
Overstin
Ovesterin
Ovestin
Ovestinon

Ovestrion
 Ovo-Vinces
 Stiptanon
 Synapause
 Theelol
 Thulol
 Tridestrin
 Trihydroxyestrin
 Trihydroxyoestrin
 Triodurin
 Trio vex

Inchi: InChI=1S/C18H24O3/c1-18-7-6-13-12-5-3-11(19)8-10(12)2-4-14(13)15(18)9-16(20)17(18)
InchiKey: PROQIPRRNZUXQM-PVGHXWSTSA-N
Formula: C18H24O3
SMILES: CC12CCC3c4ccc(O)cc4CCC3C1CC(O)C2O
Mol. weight [g/mol]: 288.38
CAS: 50-27-1

Physical Properties

Property code	Value	Unit	Source
gf	-95.37	kJ/mol	Joback Method
hf	-511.26	kJ/mol	Joback Method
hfus	37.11	kJ/mol	Joback Method
hvap	102.98	kJ/mol	Joback Method
log10ws	-4.09		Aqueous Solubility Prediction Method
log10ws	-4.96		Estimated Solubility Method
logp	2.580		Crippen Method
mcvol	225.750	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	2970.00		NIST Webbook
rinpol	2970.00		NIST Webbook
rinpol	2970.00		NIST Webbook
rinpol	2936.80		NIST Webbook
rinpol	2936.80		NIST Webbook
tb	922.87	K	Joback Method
tc	1147.96	K	Joback Method
tf	554.82	K	Aqueous Solubility Prediction Method

tf	553.20	K	Experimental solubility of diosgenin and estriol in various solvents between T = (293.2-328.2) K
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.84	J/molxK	922.87	Joback Method
cpg	835.77	J/molxK	960.38	Joback Method
cpg	855.14	J/molxK	997.90	Joback Method
cpg	875.20	J/molxK	1035.41	Joback Method
cpg	896.22	J/molxK	1072.93	Joback Method
cpg	918.44	J/molxK	1110.44	Joback Method
cpg	942.13	J/molxK	1147.96	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C50271&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Experimental solubility of diosgenin and estriol in various solvents between T = (293.2-328.2) K: <https://www.doi.org/10.1016/j.jct.2016.11.017>

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

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

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>

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

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