

Ethinyl Estradiol

Other names:

17-Ethinyl-3,17-estradiol
17-Ethinyl-3,17-oestradiol
17-Ethinylestradiol
17-Ethynyl-3-17-dihydroxy-1,3,5-oestratriene
17-Ethynylestra-1(10),2,4-triene-3,17-diol
17-Ethynylestradiol
17-Ethynylestradiol ram
17-Ethynyloestra-1,3,5(10)-triene-3,17«beta»-diol
17-Ethynyloestra-1,3,5(10)-triene-3,17Â«betaÂ»-diol
17-Ethynyloestradiol
17.alpha.-ethinyl-17.beta.-estradiol
17.alpha.-ethinylestradiol
17.alpha.-ethynylestra-1,3,5(10)-triene-3,17.beta.-diol
17.alpha.-ethynylestradiol
17«alpha»-Ethinyl-1,3,5(10)-estratriene-3,17-diol
17«alpha»-Ethinyl-17«beta»-estradiol
17«alpha»-Ethinyl-3,17-dihydroxy-«delta»(sup1,3,5)-estratriene
17«alpha»-Ethinylestra-1,3,5(10)-triene-3,17«beta»-diol
17«alpha»-Ethinylestradiol
17«alpha»-Ethinyl-1,3,5(10)-estratriene-3,17«beta»-diol
17«alpha»-Ethinyl-1,3,5(10)-oestratriene-3,17«beta»-diol
17«alpha»-Ethinyl-1,3,5-estratriene-3,17«beta»-diol
17«alpha»-Ethinyl-1,3,5-oestratriene-3,17«beta»-diol
17«alpha»-Ethinyl-17«beta»-oestradiol
17«alpha»-Ethynylestra-1,3,5(10)-triene-3,17«beta»-diol
17«alpha»-Ethynylestradiol
17«alpha»-Ethynylestradiol-17«beta»
17«alpha»-Ethynyloestra-1,3,5(10)-triene-3,17«beta»-diol
17«alpha»-Ethynyloestradiol
17«alpha»-Ethynyloestradiol-17«beta»
17«alpha»-ethinyl-3,17-dihydroxy-«delta»(sup1,3,5)oestratriene
17«alpha»-ethinyl-«delta»(sup1,3,5(10))oestratriene-3,17-«beta» -diol
17«alpha»-ethynyloestra-1,3,5(10)-triene-3,17«beta»-diol
17«beta»-Estradiol, 17-ethynyl-
17Â«alphaÂ»-Ethinyl-1,3,5(10)-estratriene-3,17-diol
17Â«alphaÂ»-Ethinyl-17Â«betaÂ»-estradiol
17Â«alphaÂ»-Ethinyl-3,17-dihydroxy-Â«deltaÂ»(sup1,3,5)-estratriene
17Â«alphaÂ»-Ethinylestra-1,3,5(10)-triene-3,17Â«betaÂ»-diol
17Â«alphaÂ»-Ethinylestradiol
17Â«alphaÂ»-Ethinyl-1,3,5(10)-estratriene-3,17Â«betaÂ»-diol

17 α -Ethynyl-1,3,5(10)-oestratriene-3,17 β -diol
 17 α -Ethynyl-1,3,5-estratriene-3,17 β -diol
 17 α -Ethynyl-1,3,5-oestratriene-3,17 β -diol
 17 α -Ethynyl-17 β -oestradiol
 17 α -Ethynylestra-1,3,5(10)-triene-3,17 β -diol
 17 α -Ethynylestradiol
 17 α -Ethynylestradiol-17 β
 17 α -Ethynyloestra-1,3,5(10)-triene-3,17 β -diol
 17 α -Ethynyloestradiol
 17 α -Ethynyloestradiol-17 β
 17 α -ethinyl-3,17-dihydroxy- Δ (sup1,3,5)estratriene
 17 α -ethinyl- Δ (sup1,3,5(10))estratriene-3,17 β -diol
 17 α -ethynyloestra-1,3,5(10)-triene-3,17 β -diol
 17 β -Estradiol, 17-ethynyl-
 19-Nor-17 α -pregna-1,3,5(10)-trien-20-yn-3,17-diol
 19-Nor-17 α -pregna-1,3,5(10)-trien-20-yne-3,17 β -diol
 19-Nor-17 α -pregna-1,3,5(10)-trien-20-yn-3,17-diol
 19-Nor-17 α -pregna-1,3,5(10)-trien-20-yne-3,17 β -diol
 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol (ethinyl estradiol)
 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17 α)-
 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17 α)-
 19-nor-17 α -pregna-1,3,5(10)-trien-20-yne-3,17-diol
 19-nor-17 α -Pregna-1,3,5(10)-trien-20-yne-3,17-diol
 19-nor-17 α -Pregna-1,3,5(10)-trien-20-yne-3,17-diol
 3,17 β -Dihydroxy-17 α -ethynyl-1,3,5(10)-estratriene
 3,17 β -Dihydroxy-17 α -ethynyl-1,3,5(10)-oestratriene
 3,17 β -Dihydroxy-17 α -ethynyl-1,3,5(10)-estratriene
 3,17 β -Dihydroxy-17 α -ethynyl-1,3,5(10)-oestratriene
 Amenoron
 Anovlar
 Chee-O-Gen
 Chee-O-Genf
 Diognat-E
 Diogyn-E
 Dyloform
 EE
 Ertonyl
 Esteed
 Estigyn
 Estinyl
 Eston-E
 Estoral
 Estoral (orion)

Estorals

Estra-1,3,5(10)-triene-3,17«beta»-diol, 17-ethynyl-

Estra-1,3,5(10)-triene-3,17«beta»-diol, 17«alpha»-ethynyl-

Estra-1,3,5(10)-triene-3,17Â«betaÂ»-diol, 17-ethynyl-

Estra-1,3,5(10)-triene-3,17Â«betaÂ»-diol, 17Â«alphaÂ»-ethynyl-

Estradiol, 17-ethynyl-

Estrogen

Ethidol

Ethinoral

Ethinylestriol

Ethinylloestradiol

Ethy 11

Ethynylestradiol

Ethynylloestradiol

Eticyclin

Eticyclol

Eticylol

Etinestrol

Etinestryl

Etinoestryl

Etistradiol

Etivex

Feminone

Follicoral

Ginestrene

Gynolett

Inestra

Kolpolyn

Linoral

Lynoral

Menolyn

NSC-10973

Neo-Estrone

Nogest-S

Novestrol

Oradiol

Orestralyn

Orestrayln

Ovex

Palonyl

Perovex

Primogyn

Primogyn C

Primogyn M
Progynon C
Progynon M
Prosexol
Spanestrin
Thiuram E
Thiuranide
Ylestol
Ylestrol
component of Brevicon
component of Demulen
component of Desogen
component of Estopherol
component of Estostep
component of Estrostep
component of Gynetone
component of Halodrin
component of Levlen
component of Lo/ovral
component of Loestrin
component of Modicon
component of Neocon
component of Nolestrin
component of Nordette
component of Norethin 1/35e
component of Norethrin 1/35e
component of Norlestrin
component of Oracon
component of Ortho-cyclen
component of Ortho-novum
component of Ortrel
component of Ovcon
component of Ovral
component of Tri-levlen
component of Triphasil
component of Zorane
ethinylestradiol

Inchi:

InChI=1S/C20H24O2/c1-3-20(22)11-9-18-17-6-4-13-12-14(21)5-7-15(13)16(17)8-10-19(14)

InchiKey:

BFPYWIDHMRZLRN-UHFFFAOYSA-N

Formula:

C₂₀H₂₄O₂

SMILES:

C#CC1(O)CCC2C3CCc4cc(O)ccc4C3CCC21C

Mol. weight [g/mol]:

296.40

CAS:

57-63-6

Physical Properties

Property code	Value	Unit	Source
gf	283.58	kJ/mol	Joback Method
hf	-72.83	kJ/mol	Joback Method
hfus	33.80	kJ/mol	Joback Method
hvap	89.77	kJ/mol	Joback Method
log10ws	-4.30		Aqueous Solubility Prediction Method
log10ws	-4.30		Estimated Solubility Method
logp	3.613		Crippen Method
mcvol	239.460	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	2782.90		NIST Webbook
rinpol	2719.00		NIST Webbook
rinpol	2719.00		NIST Webbook
tb	871.48	K	Joback Method
tc	1117.97	K	Joback Method
tf	459.00 ± 1.00	K	NIST Webbook
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.73	J/mol×K	1076.89	Joback Method
cpg	807.81	J/mol×K	871.48	Joback Method
cpg	830.60	J/mol×K	912.56	Joback Method
cpg	854.59	J/mol×K	953.64	Joback Method
cpg	880.29	J/mol×K	994.73	Joback Method
cpg	908.18	J/mol×K	1035.81	Joback Method
cpg	972.44	J/mol×K	1117.97	Joback Method
hfust	27.57	kJ/mol	456.20	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Aqueous Solubilities of Estrone, 17β-Estradiol, 17α-Ethinylestradiol, and Estriol:	https://www.doi.org/10.1021/je050318c
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57636&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
hfust:	Enthalpy of fusion at a given temperature
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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