

Ethinyl Estradiol

Other names: 17-Ethinyl-3,17-estradiol
17-Ethinyl-3,17-oestradiol
17-Ethinylestradiol
17-Ethylyn-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.-ethynylestradiol
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»-Ethynylestra-1,3,5(10)-triene-3,17«beta»-diol
17«alpha»-Ethinylestradiol
17«alpha»-Ethylyn-1,3,5(10)-estratriene-3,17«beta»-diol
17«alpha»-Ethynyl-1,3,5(10)-oestratriene-3,17«beta»-diol
17«alpha»-Ethynyl-1,3,5-estratriene-3,17«beta»-diol
17«alpha»-Ethylyn-1,3,5-oestratriene-3,17«beta»-diol
17«alpha»-Ethynyl-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»-ethinyloestra-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»-Ethynylestra-1,3,5(10)-triene-3,17Â«betaÂ»-diol
17Â«alphaÂ»-Ethynylestradiol
17Â«alphaÂ»-Ethylyn-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 -ethynloestra-1,3,5(10)-triene-3,17 β -diol
17 α -ethynloestradiol
17 α -ethynloestradiol-17 β
17 α -ethynyl-3,17-dihydroxy- δ (sup1,3,5)oestratriene
17 α -ethynyl- δ (sup1,3,5(10))oestratriene-3,17 β -diol
17 α -ethynloestra-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 β -pregna-1,3,5(10)-trien-20-yn-3,17-diol
19-Nor-17 β -pregna-1,3,5(10)-trien-20-yne-3,17 β -diol
19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol (ethynyl 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 β)-
19-nor-17 α -Pregna-1,3,5(10)-trien-20-yne-3,17-diol
19-nor-17 β -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 β -ethynyl-1,3,5(10)-estratriene
3,17 β -Dihydroxy-17 β -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
Ethinyloestradiol
Ethy 11
Ethynylestradiol
Ethynyoestradiol
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()
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	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	938.73	J/mol×K	1076.89	Joback Method
cpg	972.44	J/mol×K	1117.97	Joback Method
hfust	27.57	kJ/mol	456.20	NIST Webbook

Sources

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/ci034243xi20040112_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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
Aqueous Solubilities of Estrone, 17β-Estradiol, 17α-Ethynodiol, and Bisphenol A:	https://www.doi.org/10.1021/je050318c

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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