

Estradiol

Other names:

(+)-3,17.beta.-estradiol
(+)-3,17«beta»-Estradiol
(+)-3,17Â«betaÂ»-Estradiol
(17.beta.)-estra-1,3,5(10)-triene-3,17diol
1,3,5,(10)-Estratrien-3,17«beta»-diol
1,3,5,(10)-Estratrien-3,17Â«betaÂ»-diol
1,3,5-Estratriene-3,17«beta»-diol
1,3,5-Estratriene-3,17Â«betaÂ»-diol
17.beta.-estradiol
17.beta.-oestradiol
17«beta»-Estra-1,3,5(10)-triene-3,17-diol
17«beta»-Estradiol
17«beta»-OH-estradiol
17«beta»-OH-oestradiol
17«beta»-Oestra-1,3,5(10)-triene-3,17-diol
17«beta»-Oestradiol
17Â«betaÂ»-Estra-1,3,5(10)-triene-3,17-diol
17Â«betaÂ»-Estradiol
17Â«betaÂ»-OH-estradiol
17Â«betaÂ»-OH-oestradiol
17Â«betaÂ»-Oestra-1,3,5(10)-triene-3,17-diol
17Â«betaÂ»-Oestradiol
3,17-Epidihydroxyestratriene
3,17-Epidihydroxyestratrienelor
3,17-Epidihydroxyoestratriene
3,17-«beta»-Oestradiol
3,17-Â«betaÂ»-Oestradiol
3,17.beta.-dihydroxyestra-1,3,5(10)-triene
3,17.beta.-estradiol
3,17«beta»-Dihydroxy-1,3,5(10)-estratriene
3,17«beta»-Dihydroxy-1,3,5(10)-oestratriene
3,17«beta»-Dihydroxyestra-1,3,5(10)-triene
3,17«beta»-Dihydroxyestra-1,3,5-triene
3,17«beta»-Dihydroxyoestra-1,3,5-triene
3,17«beta»-Estradiol
3,17Â«betaÂ»-Dihydroxy-1,3,5(10)-estratriene
3,17Â«betaÂ»-Dihydroxy-1,3,5(10)-oestratriene
3,17Â«betaÂ»-Dihydroxyestra-1,3,5(10)-triene
3,17Â«betaÂ»-Dihydroxyestra-1,3,5-triene
3,17Â«betaÂ»-Dihydroxyoestra-1,3,5-triene

3,17- β -Estradiol
Agofollin
Altrad
Amnestrogen
Aquadiol
Bardiol
Benzogynestry
Beta-estradiol
Climara
Corpagen
D-3,17- β -Estradiol
D-3,17- β -Oestradiol
D-3,17- β -Estradiol
D-3,17- β -Oestradiol
D-Estradiol
D-Oestradiol
Dihydrofollicular hormone
Dihydrofolliculin
Dihydromenformon
Dihydrotheelin
Dihydroxyesterin
Dihydroxyestrin
Dihydroxyoestrin
Dimenformon
Dimenformon prolongatum
Diogyn
Diogynets
E 2
E₂
Epiestriol 50
Estasorb
Estra-1(10),2,4-triene-3,17-diol
Estra-1,3,5(10)-triene-3,17-diol (17- β)-
Estra-1,3,5(10)-triene-3,17-diol (17- β)-
Estra-1,3,5(10)-triene-3,17 β -diol
Estra-1,3,5(10)-triene-3,17- β -diol
Estra-1,3,5(10)-triene-3,17- β -diol
Estrace
Estraderm
Estraderm TTS
Estradiol, β -
Estradiol, β -
Estradiol-17- β

Estradiol-17 \hat{A} «beta \hat{A} »
Estradot
Estraldine
Estring vaginal ring
Estroclim
Estrol
Estropause
Estrovite
Evex
Evorel
Femanest
Femestral
Femestrol
Femogen
Follicyclin
Gelestra
Ginosedol
Gynergon
Gynestrel
Gynoestryl
Lamdiol
Macrodiol
Macrol
Menest
Menorest
Microdiol
NSC-20293
NSC-9895
Nordicol
Oesclim
Oestergon
Oestra-1,3,5(10)-triene-3,17«beta»-diol
Oestra-1,3,5(10)-triene-3,17 \hat{A} «beta \hat{A} »-diol
Oestradiol
Oestradiol R
Oestradiol-17«beta»
Oestradiol-17 \hat{A} «beta \hat{A} »
Oestrogel
Oestroglandol
Oestrogynol
Ovahormon
Ovasterol
Ovastevol

Ovociclina
Ovocyclin
Ovocycline
Ovocylin
Perlatanol
Primofol
Profoliol
Profoliol B
Progynon
Progynon-DH
Ricifon
Ritsifon
SK-Estrogens
Soldep
Sotipox
Syndiol
System
Theelin, dihydro-
Trocosome
Vagifem
Vivelle
Zumenon
cis-Estradiol
cis-Oestradiol
component of Menrium
estra-1,3,5(10)-triene-3,17-diol, (17.beta.)-
estra-1,3,5(10)-triene-3,17.beta.-diol
«alpha»-Estradiol
«alpha»-Oestradiol
«beta»-Estradiol
«beta»-Oestradiol
Â«alphaÂ»-Estradiol
Â«alphaÂ»-Oestradiol
Â«betaÂ»-Estradiol
Â«betaÂ»-Oestradiol

Inchi:

InChI=1S/C18H24O2/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:

VOXZDWNPVJITMN-AWDGRILASA-N

Formula:

C18H24O2

SMILES:

CC12CCC3c4ccc(O)cc4CCC3C1CCC2O

Mol. weight [g/mol]:

272.38

CAS:

50-28-2

Physical Properties

Property code	Value	Unit	Source
gf	49.16	kJ/mol	Joback Method
hf	-338.69	kJ/mol	Joback Method
hfus	31.95	kJ/mol	Joback Method
hvap	86.61	kJ/mol	Joback Method
log10ws	-5.03		Estimated Solubility Method
logp	3.609		Crippen Method
mcvol	219.880	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	2716.50		NIST Webbook
rinpol	2667.00		NIST Webbook
rinpol	2668.00		NIST Webbook
rinpol	2667.00		NIST Webbook
tb	835.36	K	Joback Method
tc	1069.90	K	Joback Method
tf	453.00 ± 1.00	K	NIST Webbook
vc	0.771	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.75	J/mol×K	835.36	Joback Method
cpg	768.05	J/mol×K	874.45	Joback Method
cpg	787.26	J/mol×K	913.54	Joback Method
cpg	806.67	J/mol×K	952.63	Joback Method
cpg	826.60	J/mol×K	991.72	Joback Method
cpg	847.32	J/mol×K	1030.81	Joback Method
cpg	869.14	J/mol×K	1069.90	Joback Method

Sources

Joback Method:

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

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=C50282&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Aqueous Solubilities of Estrone, 17 β -Estradiol, 17 α -Ethinylestradiol, 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
hvac: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mccvol: 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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