



Formula: C<sub>20</sub>H<sub>24</sub>O<sub>2</sub>

MW: 296.41

CAS: 57-63-6

MDL NUMBER: MFCD01881474

IUPAC: (1S,11S,15S,10R,14R)-14-ethynyl-15-methyltetracyclo[8.7.0.0.0]heptadeca-2,4,6-triene-5,14-diol

Smiles: c12[C@H]3(CC[C]4([C@H]([C@@H]3(Cc1cc(cc2)O))(CC[C@]4(C#C)O))C

THERAPEUTIC CATEGORY: Estrogen. In combination with progesteron as oral contraceptiver

VET THERAP CATEGORY: Estrogen

ACCEPTORS: 2

DONORS: 2

ROTATION BONDS: 2

N+O: 2

Chiral Centers: 5

LogP: 5.97

LogS: -5.01

LIPINSKI: 4

Synonyms: NOVESTROL;NEO-ESTRONE;ETHYNYLESTRADIOL;ETHINYL  
ESTRADIOL;LYNORAL;17ALPHA-ETHYNYL-DELTA1,3,5(10)-ESTRA-TRIENE-3,17BETA-DIO  
L;17ALPHA-ETHYNYLESTRADIOL;17ALPHA-ETHINYLESTRADIOL

CAS:57-63-6

MF:C20H24O2

MW:296.4

EINECS:200-342-2

Product Categories:Alcohols and Derivatives;Steroids;Acetylenes;Biochemistry;Functionalized  
Acetylenes;Hydroxysteroids;Intermediates & Fine Chemicals;Metabolites &  
Impurities;Pharmaceuticals Ethynyl estradiol

Chemical Properties: mp 182-183 C(lit.) refractive index -30 (C=0.4, Pyridine) solubility  
ethanol: 50 mg/mL, clear, slightly yellow Merck 3734

CAS DataBase Reference: 57-63-6(

CAS DataBase Reference: ) NIST Chemistry ReferenceEthynyl estradiol(57-63-6) EPA  
Substance Registry System19-Norpregna-1,3, 5(10)-trien-20-yne-3,17-diol,  
(17.alpha.)-(57-63-6) T Risk Statements 45-22 Safety Statements 53-36/37/39-45 WGK  
Germany 3 RTECS RC8925000 F 8 Hazardous Substances Data57-63-6(Hazardous  
Substances Data) 17a-Ethynyl-1,3,5(10)-estratriene-3,17b-diol Ethynyl estradiol

Usage And Synthesis:

Chemical Properties: Off-White to Light-Yellow Crystalline Powder UsageA metabolite of  
17a-Ethynylestradiol UsageA synthetic steroid with high oral estrogenic potency General  
DescriptionFine white to creamy white powder. A synthetic steroid. Used in combination with  
progestogen as an oral contraceptive. Air & Water ReactionsAir and light sensitive . Insoluble in  
water. Reactivity ProfileEthynyl estradiol may react vigorously with strong oxidizing agents. May  
react exothermically with reducing agents to generate gaseous hydrogen. Health  
HazardACUTE/CHRONIC HAZARDS: When heated to decomposition Ethynyl estradiol emits  
acid smoke- and fumes. Fire HazardThe flash point data for Ethynyl estradiol are not available.  
Ethynyl estradiol is probably combustible. Ethynyl estradiol

