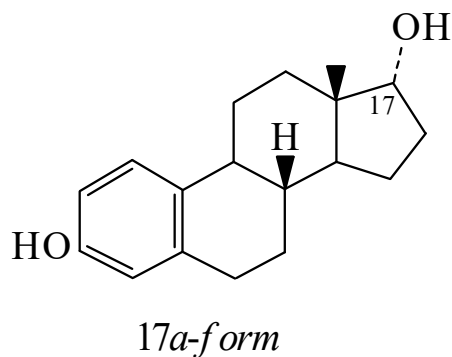




>>Entry Name: Estra-1,3,5(10)-triene-3,17-diol



Molecular Formula: C₁₈H₂₄O₂

Molecular Weight: 272.386

Accurate Mass: 272.17763

Percentage Composition: C 79.37%; H 8.88%; O 11.75%

General Statement: Estradiol is the accepted U.S. and IUPAC spelling

>>Variant: 17 α -form

Synonym(s): Estradiol-17 α . β -Estradiol (obsol., misleading). Epiestradiol. Alfatradiol, INN

CAS Registry Number: 57-91-0

Molecular Formula: C₁₈H₂₄O₂

Molecular Weight: 272.386

Accurate Mass: 272.17763

Percentage Composition: C 79.37%; H 8.88%; O 11.75%

Biological Source: Isol. from pregnancy urine

Biological Use/Importance: Topical inhibitor of 5 α -reductase

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 223°

Optical Rotation: [α]_D¹⁸+56.7 (EtOH)

Other Data: Less potent estrogen than the 17 β -isomer

Hazard & Toxicity: Exp. reprod. effects

Aldrich: 28577-3

Sigma: E8750

>>Derivative: Di-Ac

CAS Registry Number: 1474-52-8

Molecular Formula: C₂₂H₂₈O₄

Molecular Weight: 356.461

Accurate Mass: 356.19876

Percentage Composition: C 74.13%; H 7.92%; O 17.95%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 139-140°

>>Variant: 17 β -form

Synonym(s): Estradiol, INN, USAN. Oestradiol, BAN. α -Estradiol (obsol., misleading). Almediol. Alora. Climara. Climaval. Compudose. Dermestril. Elleste-solo. Estrace. Estraderm. Evoral. Fematrix. FemSeven. Menorest. Oestrogel. Ovocyclin. Progynova. Sandrena. Vagifem. Zumenon. Many other names

CAS Registry Number: 50-28-2

Molecular Formula: C₁₈H₂₄O₂

Molecular Weight: 272.386

Accurate Mass: 272.17763

Percentage Composition: C 79.37%; H 8.88%; O 11.75%

Biological Source: Isol. from ovaries and pregnancy urine. Sex pheromone for mallard ducks

Biological Use/Importance: The most potent of the natural estrogens. Estradiol (and its semisynthetic esters) are used in estrogen replacement therapy

Physical Description: Leaflets or needles (EtOH aq.)

Development Status: Marketed drug

Melting Point: Mp 178°

Optical Rotation: [α]_D¹⁸+78 (EtOH)

Calculated Log P Data: Log P 3.78 (uncertain value) (calc)

Hazard & Toxicity: Exp. carcinogen. Human and exp. reprod. effects. Exp. teratogenic effects. Semisynthetic esters should be considered to have similar toxicological properties