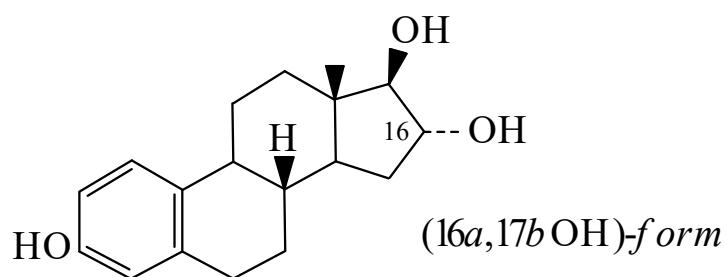




>>Entry Name: Estra-1,3,5(10)-triene-3,16,17-triol



Related CAS Registry Numbers(s): 113-22-4

Molecular Formula: $C_{18}H_{24}O_3$

Molecular Weight: 288.386

Accurate Mass: 288.172545

Percentage Composition: C 74.97%; H 8.39%; O 16.64%

>>Variant: (16 α ,17 α OH)-form

Synonym(s): 17-Epiestriol

CAS Registry Number: 1228-72-4

Molecular Formula: $C_{18}H_{24}O_3$

Molecular Weight: 288.386

Accurate Mass: 288.172545

Percentage Composition: C 74.97%; H 8.39%; O 16.64%

Biological Source: Present in urine in pregnancy

Melting Point: Mp 230-235°

Sigma: E3750

>>Derivative: 16,17-Di-Ac

Molecular Formula: $C_{22}H_{28}O_5$

Molecular Weight: 372.46

Accurate Mass: 372.193675

Percentage Composition: C 70.95%; H 7.58%; O 21.48%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 193-195°

>>Derivative: Tri-Ac

CAS Registry Number: 2236-33-1

Molecular Formula: $C_{24}H_{30}O_6$

Molecular Weight: 414.497

Accurate Mass: 414.20424

Percentage Composition: C 69.55%; H 7.29%; O 23.16%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 162-164°

>>Derivative: 3-Me ether

Synonym(s): 3-Methoxyestra-1,3,5(10)-triene-16 α ,17 α -diol, 9Cl, 8Cl. **Epimestrol**, BAN, INN, USAN. Alene. Stimoval. NSC 55975. Org 817

CAS Registry Number: 7004-98-0

Molecular Formula: $C_{19}H_{26}O_3$

Molecular Weight: 302.413

Accurate Mass: 302.188195

Percentage Composition: C 75.46%; H 8.67%; O 15.87%

Use/Importance: Estrogen, anterior pituitary activator

Melting Point: Mp 158-160°

Optical Rotation: $[\alpha]_D^{20} +48$ (CHCl₃)

Calculated Log P Data: Log P 3.14 (uncertain value) (calc)