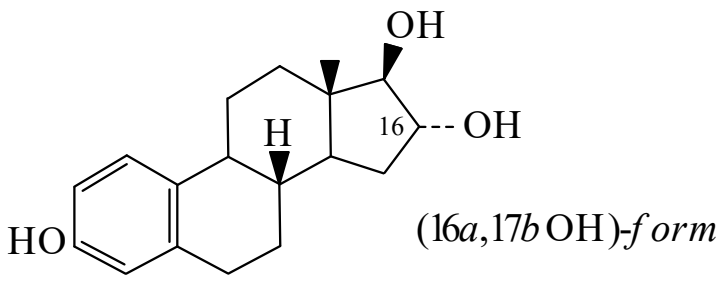
>>**Entry Name: Estra-1,3,5(10)-triene-3,16,17-triol**



(16*a*,17*b* OH)-*form*

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:** (16α,17αOH)-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. (Et_2O)
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-16α,17α-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 ($CHCl_3$)
Calculated Log P Data: Log P 3.14 (uncertain value) (calc)