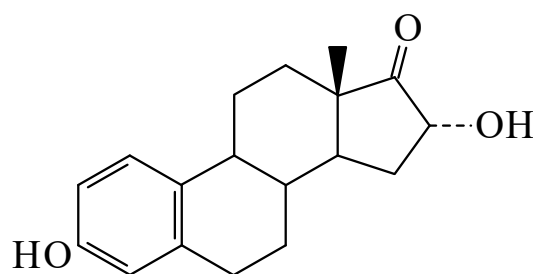




>>Entry Name: 3,16-Dihydroxyestra-1,3,5(10)-trien-17-one, 9CI

Synonym(s): 16-Hydroxyestrone



Related CAS Registry Numbers(s): 18186-49-7 20796-71-8 62013-81-4 80225-93-0 86790-92-3

Molecular Formula: C₁₈H₂₂O₃

Molecular Weight: 286.37

Accurate Mass: 286.156895

Percentage Composition: C 75.50%; H 7.74%; O 16.76%

>>Variant: 16 α -form

CAS Registry Number: 566-76-7

Molecular Formula: C₁₈H₂₂O₃

Molecular Weight: 286.37

Accurate Mass: 286.156895

Percentage Composition: C 75.50%; H 7.74%; O 16.76%

Physical Description: Plates (MeOH)

Melting Point: Mp 205-207°

Optical Rotation: $[\alpha]_D^{28} +168.8$ (EtOH)

Sigma: H8004

>>Derivative: Di-Ac

Synonym(s): 3,16 α -Diacetoxyestra-1,3,5(10)-trien-17-one. Colpogynon. Colpormon

CAS Registry Number: 1247-71-8

Molecular Formula: C₂₂H₂₆O₅

Molecular Weight: 370.444

Accurate Mass: 370.178025

Percentage Composition: C 71.33%; H 7.07%; O 21.59%

Use/Importance: Estrogen

Physical Description: Plates (EtOH)

Melting Point: Mp 174°

Optical Rotation: $[\alpha]_D^{28} +122$ (CHCl₃)

>>Derivative: 3-Me ether

Synonym(s): 16 α -Hydroxy-3-methoxyestra-1,3,5(10)-trien-17-one

CAS Registry Number: 3434-77-3

Molecular Formula: C₁₉H₂₄O₃

Molecular Weight: 300.397

Accurate Mass: 300.172545

Percentage Composition: C 75.97%; H 8.05%; O 15.98%

Melting Point: Mp 156-157°

Optical Rotation: $[\alpha]_D +176$ (CHCl₃)

>>Derivative: Di-Me ether

Synonym(s): 3,16 α -Dimethoxyestra-1,3,5(10)-trien-17-one

Molecular Formula: C₂₀H₂₆O₃

Molecular Weight: 314.424

Accurate Mass: 314.188195

Percentage Composition: C 76.40%; H 8.33%; O 15.27%

Physical Description: Prisms (MeOH)

Melting Point: Mp 96-97.5°