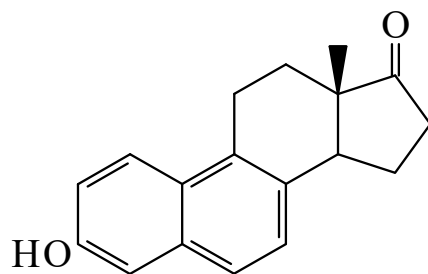




>>Entry Name: 3-Hydroxyestra-1,3,5,7,9-pentaen-17-one, 9CI



CAS Registry Number: 517-09-9

Molecular Formula: C₁₈H₁₈O₂

Molecular Weight: 266.339

Accurate Mass: 266.13068

Percentage Composition: C 81.17%; H 6.81%; O 12.01%

Sigma: E0627

>>Variant: (+)-form

Synonym(s): Equilenin

Molecular Formula: C₁₈H₁₈O₂

Molecular Weight: 266.339

Accurate Mass: 266.13068

Percentage Composition: C 81.17%; H 6.81%; O 12.01%

Biological Source: Constit. of urine of pregnant mares

Use/Importance: Estrogen

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 258-259° (250-251°)

Optical Rotation: $[\alpha]_D^{16} +87$ (dioxan)

Calculated Log P Data: Log P 3.12 (calc)

Other Data: Mp in open tubes variable due to oxidn.

Hazard & Toxicity: Exp. reprod. effects

>>Derivative: Oxime

Molecular Formula: C₁₈H₁₉NO₂

Molecular Weight: 281.354

Accurate Mass: 281.141579

Percentage Composition: C 76.84%; H 6.81%; N 4.98%; O 11.37%

Melting Point: Mp 249-250°

>>Derivative: Semicarbazone

Melting Point: Mp 268°

>>Derivative: Ac

CAS Registry Number: 6030-91-7

Molecular Formula: C₂₀H₂₀O₃

Molecular Weight: 308.376

Accurate Mass: 308.141245

Percentage Composition: C 77.90%; H 6.54%; O 15.56%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 157-158°

Optical Rotation: $[\alpha]_D^{20} +72$ (CHCl₃)

>>Derivative: Benzoyl

CAS Registry Number: 604-58-0

Melting Point: Mp 222-223°

Hazard & Toxicity: Exp. neoplastic agent. Exp. reprod. effects