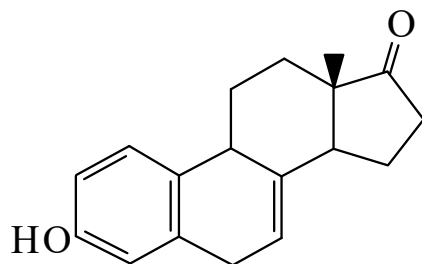




>>Entry Name: 3-Hydroxyestra-1,3,5(10),7-tetraen-17-one, 9CI

Synonym(s): Equilin



CAS Registry Number: 474-86-2

Related CAS Registry Numbers(s): 23962-01-8 43085-97-8

Molecular Formula: C₁₈H₂₀O₂

Molecular Weight: 268.355

Accurate Mass: 268.14633

Percentage Composition: C 80.56%; H 7.51%; O 11.92%

Biological Source: Obt. from urine of pregnant mares

Use/Importance: Estrogen

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 238-240°

Optical Rotation: [α]_D²⁵+325 (c, 2 in EtOH). [α]_D+308 (CHCl₃)

Calculated Log P Data: Log P 2.9 (uncertain value) (calc)

Hazard & Toxicity: Exp. neoplastic agent

Sigma: E8126

>>Derivative: Me ether

Synonym(s): 3-Methoxyestra-1,3,5(10),7-tetraen-17-one

CAS Registry Number: 6030-83-7

Molecular Formula: C₁₉H₂₂O₂

Molecular Weight: 282.382

Accurate Mass: 282.16198

Percentage Composition: C 80.82%; H 7.85%; O 11.33%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 161-163°

Optical Rotation: [α]_D+290 (c, 1 in CHCl₃)

Sigma: E9380

>>Variant: (±)-form

CAS Registry Number: 24022-60-4

Molecular Formula: C₁₈H₂₀O₂

Molecular Weight: 268.355

Accurate Mass: 268.14633

Percentage Composition: C 80.56%; H 7.51%; O 11.92%

Physical Description: Cryst. (2-propanol)

Melting Point: Mp 222-224°

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