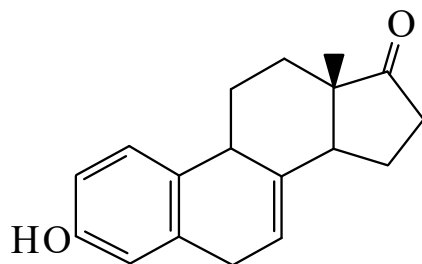




>>Entry Name: 3-Hydroxyestra-1,3,5(10),7-tetraen-17-one, 9CI

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: $[\alpha]_D^{25} +325$ (c, 2 in EtOH). $[\alpha]_D +308$ (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: $[\alpha]_D +290$ (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°

References:

Zderic, J.A. *et al.*, *J.A.C.S.*, 1958, **80**, 2596-2597, (*synth, uv*)

Zderic, J.A. *et al.*, *Steroids*, 1963, **1**, 233-249, (*synth, uv*)

Marshall, D.J. *et al.*, *Can. J. Chem.*, 1969, **47**, 3127-3131, (*synth*)

Stein, R.P. *et al.*, *Tetrahedron*, 1970, **26**, 1917-1933, (*synth, bibl, uv*)

Bhavnani, B.R. *et al.*, *Endocrinology (Baltimore)*, 1973, **92**, 1397-1404, (*biosynth*)

Smith, D.H. *et al.*, *Tetrahedron*, 1973, **29**, 3117-3134, (*ms*)

Taub, D., *The Total Synthesis of Natural Products*, (ed. ApSimon, J.W.), Wiley, 1973, **2**, 664-670, (*rev*)

Bhavnani, B.R. *et al.*, *J. Steroid Biochem.*, 1982, **17**, 217-223, (*metab*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1183

Sawicki, M.W. *et al.*, *Acta Cryst. C*, 1999, **55**, 425-427, (*cryst struct*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, ECW000*