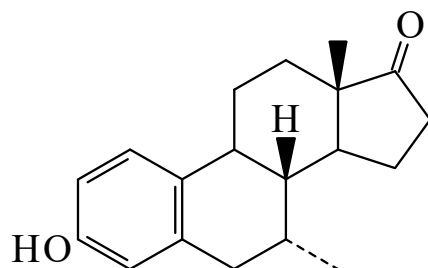




>>Entry Name: 3-Hydroxy-7-methylestra-1,3,5(10)-trien-17-one, 9Cl



Related CAS Registry Numbers(s): 32297-40-8 32344-14-2 36014-09-2 69260-11-3

Molecular Formula: C₁₉H₂₄O₂

Molecular Weight: 284.397

Accurate Mass: 284.17763

Percentage Composition: C 80.24%; H 8.51%; O 11.25%

>>Variant: 7 α -form

Synonym(s): Alimestrone, INN. 7 α -Methylestrone. Ba 38372. Ciba 38372

CAS Registry Number: 10448-96-1

Molecular Formula: C₁₉H₂₄O₂

Molecular Weight: 284.397

Accurate Mass: 284.17763

Percentage Composition: C 80.24%; H 8.51%; O 11.25%

Use/Importance: Estrogen

Physical Description: Cryst. (CH₂Cl₂/MeOH)

Melting Point: Mp 237-238°

Optical Rotation: $[\alpha]_D^{20} +149$ (c, 1.186 in CHCl₃)

Calculated Log P Data: Log P 3.9 (uncertain value) (calc)

>>Derivative: Me ether

Synonym(s): 3-Methoxy-7 α -methylestra-1,3,5(10)-trien-17-one

CAS Registry Number: 10449-00-0

Molecular Formula: C₂₀H₂₆O₂

Molecular Weight: 298.424

Accurate Mass: 298.19328

Percentage Composition: C 80.50%; H 8.78%; O 10.72%

Physical Description: Cryst. (CH₂Cl₂/MeOH)

Melting Point: Mp 163-165°

Optical Rotation: $[\alpha]_D^{16} +144$ (c, 0.477 in CHCl₃)

>>Variant: (7 β ,14 β)-form

CAS Registry Number: 60895-84-3

Molecular Formula: C₁₉H₂₄O₂

Molecular Weight: 284.397

Accurate Mass: 284.17763

Percentage Composition: C 80.24%; H 8.51%; O 11.25%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 208°

Optical Rotation: $[\alpha]_D +59$ (c, 1 in CHCl₃)

>>Variant: ($\pm$)-7 α -form

Molecular Formula: C₁₉H₂₄O₂

Molecular Weight: 284.397

Accurate Mass: 284.17763

Percentage Composition: C 80.24%; H 8.51%; O 11.25%

>>Derivative: Me ether

CAS Registry Number: 68383-37-9

Physical Description: Cryst. (MeOH)

Melting Point: Mp 144-146°