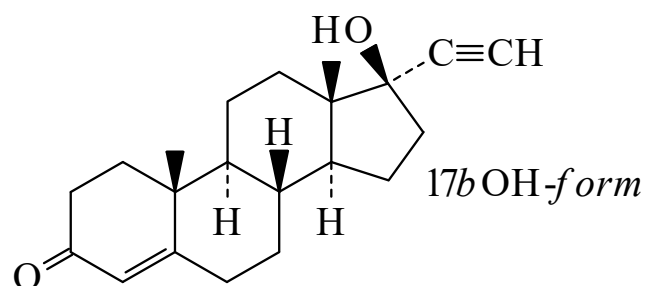




>>Entry Name: 17-Hydroxypregn-4-en-20-yn-3-one



Related CAS Registry Numbers(s): 8015-29-0

Molecular Formula: C₂₁H₂₈O₂

Molecular Weight: 312.451

Accurate Mass: 312.20893

Percentage Composition: C 80.73%; H 9.03%; O 10.24%

>>Variant: 17βOH-form

Synonym(s): Ethisterone, BAN, INN. Ethnyltestosterone. 17-Ethnyltestosterone. Ethnyltestosterone. Pregneninolone. Pregnin. Many other names

CAS Registry Number: 434-03-7

Molecular Formula: C₂₁H₂₈O₂

Molecular Weight: 312.451

Accurate Mass: 312.20893

Percentage Composition: C 80.73%; H 9.03%; O 10.24%

Biological Use/Importance: Orally effective progestational steroid, about one-third the activity of progesterone by subcutaneous route but more active orally

Physical Description: Cryst. (CHCl₃/Me₂CO or EtOAc), needles (EtOH)

Melting Point: Mp 270-272°

Optical Rotation: [α]_D²⁰+22.5 (dioxan)

Calculated Log P Data: Log P 3.81 (uncertain value) (calc)

Aldrich: 28581-1

Sigma: E1001

>>Variant: (13α,17αOH)-form

CAS Registry Number: 17554-63-1

Molecular Formula: C₂₁H₂₈O₂

Molecular Weight: 312.451

Accurate Mass: 312.20893

Percentage Composition: C 80.73%; H 9.03%; O 10.24%

Physical Description: Prisms (Me₂CO)

Melting Point: Mp 189.5-191°

Optical Rotation: [α]_D¹⁸+125 (c, 0.11 in CHCl₃)

>>Variant: (13α,17βOH)-form

CAS Registry Number: 41460-94-0

Molecular Formula: C₂₁H₂₈O₂

Molecular Weight: 312.451

Accurate Mass: 312.20893

Percentage Composition: C 80.73%; H 9.03%; O 10.24%

Physical Description: Needles (Me₂CO)

Melting Point: Mp 174-174.5°

Optical Rotation: [α]_D¹⁸+65.2 (c, 0.14 in CHCl₃)

>>Variant: (9β,10α,17α)-form

Molecular Formula: C₂₁H₂₈O₂

Molecular Weight: 312.451

Accurate Mass: 312.20893

Percentage Composition: C 80.73%; H 9.03%; O 10.24%

Melting Point: Mp 195-196°

Optical Rotation: [α]_D²⁰-219 (CHCl₃)

References: