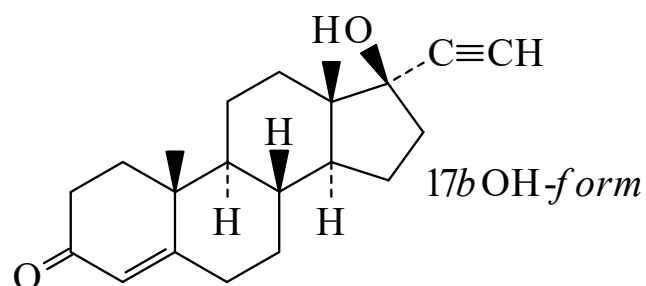




>>Entry Name: 17-Hydroxypregn-4-en-20-yn-3-one



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

**Molecular Formula:** C<sub>21</sub>H<sub>28</sub>O<sub>2</sub>

**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:** C<sub>21</sub>H<sub>28</sub>O<sub>2</sub>

**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. (CHCl<sub>3</sub>/Me<sub>2</sub>CO or EtOAc), needles (EtOH)

**Melting Point:** Mp 270-272°

**Optical Rotation:** [α]<sub>D</sub><sup>20</sup>+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:** C<sub>21</sub>H<sub>28</sub>O<sub>2</sub>

**Molecular Weight:** 312.451

**Accurate Mass:** 312.20893

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

**Physical Description:** Prisms (Me<sub>2</sub>CO)

**Melting Point:** Mp 189.5-191°

**Optical Rotation:** [α]<sub>D</sub><sup>18</sup>+125 (c, 0.11 in CHCl<sub>3</sub>)

>>Variant: (13α,17βOH)-form

**CAS Registry Number:** 41460-94-0

**Molecular Formula:** C<sub>21</sub>H<sub>28</sub>O<sub>2</sub>

**Molecular Weight:** 312.451

**Accurate Mass:** 312.20893

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

**Physical Description:** Needles (Me<sub>2</sub>CO)

**Melting Point:** Mp 174-174.5°

**Optical Rotation:** [α]<sub>D</sub><sup>18</sup>+65.2 (c, 0.14 in CHCl<sub>3</sub>)

>>Variant: (9β,10α,17α)-form

**Molecular Formula:** C<sub>21</sub>H<sub>28</sub>O<sub>2</sub>

**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]<sub>D</sub><sup>20</sup>-219 (CHCl<sub>3</sub>)

**References:**