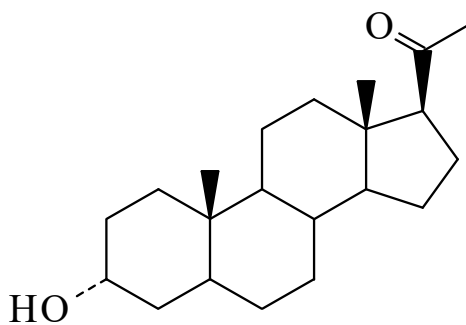




>>Entry Name: 3-Hydroxypregnan-20-one, 9Cl



CAS Registry Number: 4406-35-3

Related CAS Registry Numbers(s): 1491-77-6 4469-03-8 21788-58-9 26961-00-2 58701-70-5

Molecular Formula: C<sub>21</sub>H<sub>34</sub>O<sub>2</sub>

Molecular Weight: 318.498

Accurate Mass: 318.25588

Percentage Composition: C 79.19%; H 10.76%; O 10.05%

Solubility: BERDY SOL: Sol. MeOH, CHCl<sub>3</sub>; fairly sol. C<sub>6</sub>H<sub>6</sub>; poorly sol. H<sub>2</sub>O, hexane

UV: [neutral] λ<sub>max</sub> 262 (ε 4626); 269 (ε 4064); 303 (ε 8853) (EtOH) (Berdy)

Hazard & Toxicity: BERDY HAZD : LD<sub>50</sub> (mus, ipr) 1000 mg/kg

>>Variant: (3α,5α)-form

CAS Registry Number: 516-54-1

Molecular Formula: C<sub>21</sub>H<sub>34</sub>O<sub>2</sub>

Molecular Weight: 318.498

Accurate Mass: 318.25588

Percentage Composition: C 79.19%; H 10.76%; O 10.05%

Physical Description: Needles (Et<sub>2</sub>O)

Melting Point: Mp 175-176°

Optical Rotation: [α]<sub>D</sub><sup>24</sup>+99.7 (c, 2.2 in CHCl<sub>3</sub>)

Fluka: 81572

Sigma: P5761

>>Derivative: Ac

Molecular Formula: C<sub>23</sub>H<sub>36</sub>O<sub>3</sub>

Molecular Weight: 360.536

Accurate Mass: 360.266445

Percentage Composition: C 76.62%; H 10.06%; O 13.31%

Physical Description: Needles (Et<sub>2</sub>O)

Melting Point: Mp 141-142°

Optical Rotation: [α]<sub>D</sub><sup>24</sup>+93.1 (c, 2.1 in CHCl<sub>3</sub>)

>>Variant: (3α,5β)-form

Synonym(s): Pregnanolone. Eltanolone, INN

CAS Registry Number: 128-20-1

Molecular Formula: C<sub>21</sub>H<sub>34</sub>O<sub>2</sub>

Molecular Weight: 318.498

Accurate Mass: 318.25588

Percentage Composition: C 79.19%; H 10.76%; O 10.05%

Use/Importance: Anaesthetic

Physical Description: Cryst. (CH<sub>2</sub>Cl<sub>2</sub>/hexane)

Melting Point: Mp 150-151°

Optical Rotation: [α]<sub>D</sub><sup>23</sup>+104.6 (c, 1 in CHCl<sub>3</sub>)

Calculated Log P Data: Log P 4.51 (uncertain value) (calc)

Sigma: P8129

>>Derivative: Ac

CAS Registry Number: 1491-77-6

Melting Point: Mp 101-102°