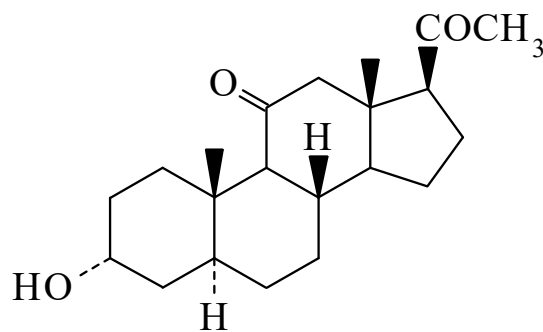




>>Entry Name: 3-Hydroxypregnane-11,20-dione, 9CI



Related CAS Registry Numbers(s): 3684-81-9 8067-82-1 16472-72-3 82597-79-3

Molecular Formula:  $C_{21}H_{32}O_3$

Molecular Weight: 332.482

Accurate Mass: 332.235145

Percentage Composition: C 75.86%; H 9.70%; O 14.44%

>>Variant: (3 $\alpha$ ,5 $\alpha$ )-form

Synonym(s): Alfaxalone, INN, JAN. Alphaxalone, BAN

CAS Registry Number: 23930-19-0

Molecular Formula:  $C_{21}H_{32}O_3$

Molecular Weight: 332.482

Accurate Mass: 332.235145

Percentage Composition: C 75.86%; H 9.70%; O 14.44%

Biological Source: Semisynthetic steroid prod. from 5 $\alpha$ -pregnane-3,11,20-trione by incubating with *Saccharomyces cerevisiae*

Use/Importance: General anaesthetic

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

Melting Point: Mp 172-174°

Optical Rotation:  $[\alpha]_D^{26} +113.4$  (c, 1.2 in CHCl<sub>3</sub>)

Calculated Log P Data: Log P 2.02 (uncertain value) (calc)

Sigma: P5052

>>Derivative: Ac

CAS Registry Number: 51267-69-7

Molecular Formula:  $C_{23}H_{34}O_4$

Molecular Weight: 374.519

Accurate Mass: 374.24571

Percentage Composition: C 73.76%; H 9.15%; O 17.09%

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

Melting Point: Mp 155-156°

Optical Rotation:  $[\alpha]_D^{24} +111$  (c, 1.77 in CHCl<sub>3</sub>)

>>Derivative: Compd. with alfadolone acetate (3:1)

Synonym(s): Alfadione. Alphadione. Alfathesin. Althesin. Aurantex. Saffan

**Hazard & Toxicity:** LD<sub>50</sub> (mus, ivn) 54.7 mg/kg

>>Variant: (3 $\alpha$ ,5 $\beta$ )-form

Synonym(s): Renanolone, INN

CAS Registry Number: 565-99-1

Molecular Formula:  $C_{21}H_{32}O_3$

Molecular Weight: 332.482

Accurate Mass: 332.235145

Percentage Composition: C 75.86%; H 9.70%; O 14.44%

Biological Source: Semisynthetic steroid prod. from 5 $\beta$ -pregnane-3,11,20-trione by incubating with *Saccharomyces cerevisiae*

Use/Importance: Anaesthetic

Physical Description: Cryst. (C<sub>6</sub>H<sub>6</sub>/Et<sub>2</sub>O)

Melting Point: Mp 168-171°