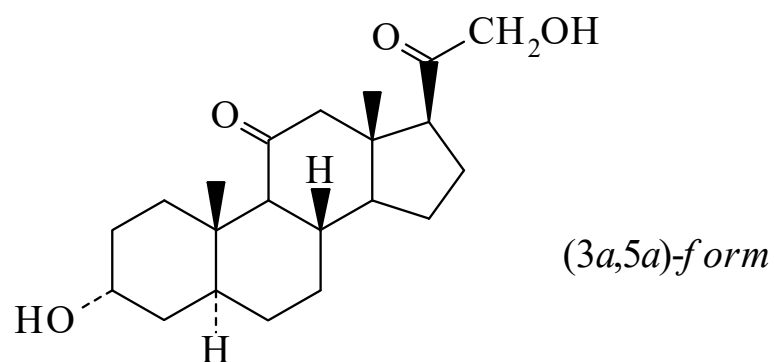




>>Entry Name: 3,21-Dihydroxypregnane-11,20-dione, 9CI



Related CAS Registry Numbers(s): 8067-82-1 38601-29-5 66829-97-8

Molecular Formula: C₂₁H₃₂O₄

Molecular Weight: 348.481

Accurate Mass: 348.23006

Percentage Composition: C 72.38%; H 9.26%; O 18.36%

>>Variant: (3α,5α)-form

Synonym(s): Alphadolone, BAN. **Alfadalone**, INN. GR 2/1574

CAS Registry Number: 14107-37-0

Type of Compound Code(s): XA0550

Molecular Formula: C₂₁H₃₂O₄

Molecular Weight: 348.481

Accurate Mass: 348.23006

Percentage Composition: C 72.38%; H 9.26%; O 18.36%

Use/Importance: Anaesthetic

Physical Description: Cryst. (Me₂CO/petrol)

Melting Point: Mp 167-170°

Optical Rotation: [α]_D²⁴ +99 (MeOH)

Calculated Log P Data: Log P 1.5 (uncertain value) (calc)

Hazard & Toxicity: LD₅₀ (mus, ivn) 59 mg/kg

>>Derivative: 21-Ac

CAS Registry Number: 23930-37-2

Molecular Formula: C₂₃H₃₄O₅

Molecular Weight: 390.519

Percentage Composition: C 70.74%; H 8.78%; O 20.48%

Use/Importance: Anaesthetic, freq. used in combination with Alfaxalone in 3-Hydroxypregnane-11,20-dione [HLQ58-U](#)

Physical Description: Cryst. (Me₂CO/hexane)

Melting Point: Mp 175-177°

Optical Rotation: [α]_D +97 (c, 1.02 in CHCl₃)

>>Variant: (3α,5β)-form

CAS Registry Number: 566-03-0

Type of Compound Code(s): VT0450 AJ0450

Molecular Formula: C₂₁H₃₂O₄

Molecular Weight: 348.481

Accurate Mass: 348.23006

Percentage Composition: C 72.38%; H 9.26%; O 18.36%

Biological Source: Present in urine

Physical Description: Cryst. (Me₂CO/hexane)

Melting Point: Mp 222-228°

Optical Rotation: [α]_D +129 (c, 1 in MeOH)

Sigma: P8272