



>>Entry Name: Pregna-4,16-diene-3,20-dione, 9Cl

Synonym(s): 16,17-Didehydropregesterone

CAS Registry Number: 1096-38-4

Molecular Formula: C₂₁H₂₈O₂

Molecular Weight: 312.451

Accurate Mass: 312.20893

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

Source/Synthesis: Synth. progestin

Physical Description: Cryst. (Me₂CO/hexane)

Melting Point: Mp 190-192°

Optical Rotation: [α]_D²³+135 (c, 0.5 in CHCl₃)

Other Data: Has only about 1% of the activity of progesterone

Aldrich: D420-2

Sigma: D5250

>>Variant: (9β,10α)-form

CAS Registry Number: 4076-95-3

Molecular Formula: C₂₁H₂₈O₂

Molecular Weight: 312.451

Accurate Mass: 312.20893

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

Physical Description: Cryst. (MeOH)

Melting Point: Mp 165-167°

>>Variant: (±)-form

CAS Registry Number: 19504-64-4

Molecular Formula: C₂₁H₂₈O₂

Molecular Weight: 312.451

Accurate Mass: 312.20893

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

Physical Description: Cryst. (C₆H₆/hexane)

Melting Point: Mp 182-184°

References:

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van der Waard, W.F. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1966, **85**, 712, (synth, uv, ir, 9β,10α-form)

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Adam, G. *et al.*, *Z. Chem.*, 1986, **26**, 369, (synth)

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