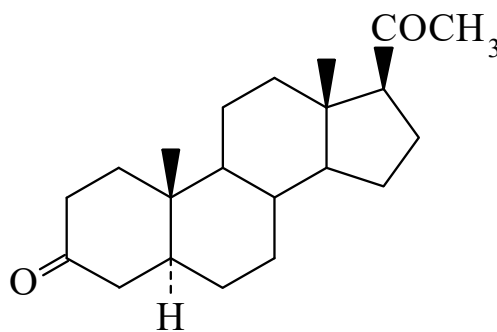




>>Entry Name: Pregnane-3,20-dione



Related CAS Registry Numbers(s): 14957-73-4 51154-66-6 51154-68-8 76094-56-9 76094-57-0 98301-13-4

Molecular Formula: C₂₁H₃₂O₂

Molecular Weight: 316.483

Accurate Mass: 316.24023

Percentage Composition: C 79.70%; H 10.19%; O 10.11%

>>Variant: 5 α -form

CAS Registry Number: 566-65-4

Molecular Formula: C₂₁H₃₂O₂

Molecular Weight: 316.483

Accurate Mass: 316.24023

Percentage Composition: C 79.70%; H 10.19%; O 10.11%

Source/Synthesis: Semisynthetic steroid prod. from pregn-4-ene-3,20-dione by incubating with *Cortinarius evernius*, *Mycobacterium smegmatis*, *Ophiobolus herpotrichus* or *Penicillium urticae*

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 198-201°

Optical Rotation: [α]_D²⁸ +121 (c, 1.038 in CHCl₃)

Sigma: P7754

>>Derivative: 3-Oxime

CAS Registry Number: 6750-73-8

Molecular Formula: C₂₁H₃₃NO₂

Molecular Weight: 331.497

Accurate Mass: 331.251129

Percentage Composition: C 76.09%; H 10.03%; N 4.23%; O 9.65%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 240-241.5°

Optical Rotation: [α]_D²⁵ +107 (c, 0.49 in CHCl₃)

>>Derivative: 20-Oxime

CAS Registry Number: 6690-25-1

Melting Point: Mp 229-232°

>>Derivative: Dioxime

Molecular Formula: C₂₁H₃₄N₂O₂

Molecular Weight: 346.512

Accurate Mass: 346.262028

Percentage Composition: C 72.79%; H 9.89%; N 8.08%; O 9.23%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 250-252 dec.°

>>Variant: 5 β -form

CAS Registry Number: 128-23-4

Molecular Formula: C₂₁H₃₂O₂

Molecular Weight: 316.483

Accurate Mass: 316.24023

Percentage Composition: C 79.70%; H 10.19%; O 10.11%

Biological Source: Constit. of human and mare's pregnancy urine. Also prepd. semisynthetically from pregn-4-ene-3,20-dione by incubating with *Alternaria bataticola* or *Bacillus putrificus*