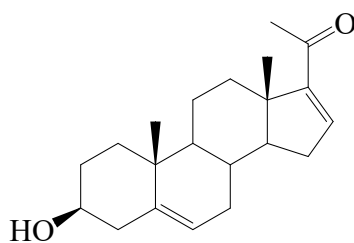




>>Entry Name: 3-Hydroxypregna-5,16-dien-20-one



Related CAS Registry Numbers(s): 23549-24-8 23549-26-0

Molecular Formula: C₂₁H₃₀O₂

Molecular Weight: 314.467

Accurate Mass: 314.22458

Percentage Composition: C 80.21%; H 9.62%; O 10.18%

>>Variant: 3β-form

CAS Registry Number: 1162-53-4

Molecular Formula: C₂₁H₃₀O₂

Molecular Weight: 314.467

Accurate Mass: 314.22458

Percentage Composition: C 80.21%; H 9.62%; O 10.18%

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 210-212°

Optical Rotation: [α]_D −34 (c, 1 in CHCl₃/dioxan)

>>Derivative: Oxime

CAS Registry Number: 23549-27-1

Molecular Formula: C₂₁H₃₁NO₂

Molecular Weight: 329.481

Accurate Mass: 329.235479

Percentage Composition: C 76.55%; H 9.48%; N 4.25%; O 9.71%

Physical Description: Needles (AcOH aq.)

Melting Point: Mp 219-220°

>>Derivative: Semicarbazone

Physical Description: Cryst. (EtOH)

Melting Point: Mp 230° (dec.)

>>Derivative: Thiosemicarbazone

Physical Description: Cryst. (EtOH)

Melting Point: Mp 242°

>>Derivative: Ac

CAS Registry Number: 979-02-2

Molecular Formula: C₂₃H₃₂O₃

Molecular Weight: 356.504

Accurate Mass: 356.235145

Percentage Composition: C 77.49%; H 9.05%; O 13.46%

Use/Importance: Key intermed. in the conversion of diosgenin to progesterone

Physical Description: Rods (MeOH)

Melting Point: Mp 175-177°

Optical Rotation: [α]_D −39 (c, 1 in CHCl₃)

>>Derivative: Ac, oxime

CAS Registry Number: 2174-13-2

Molecular Formula: C₂₃H₃₃NO₃

Molecular Weight: 371.519

Accurate Mass: 371.246044

Percentage Composition: C 74.36%; H 8.95%; N 3.77%; O 12.92%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 228-230°