



>>Entry Name: Pregnane-3,20-diol, 9CI

CAS Registry Number: 4479-11-2

Related CAS Registry Numbers(s): 567-03-3 25908-35-4 73745-18-3

Extra CAS Registry Numbers(s): 26445-07-8

Molecular Formula: C₂₁H₃₆O₂

Molecular Weight: 320.514

Accurate Mass: 320.27153

Percentage Composition: C 78.70%; H 11.32%; O 9.98%

>>Variant: (3 α ,5 α ,20*R*)-form

CAS Registry Number: 566-57-4

Molecular Formula: C₂₁H₃₆O₂

Molecular Weight: 320.514

Accurate Mass: 320.27153

Percentage Composition: C 78.70%; H 11.32%; O 9.98%

Source/Synthesis: Constit. of human pregnancy urine

Physical Description: Needles (Me₂CO)

Melting Point: Mp 207-209°

Optical Rotation: [α]_D²⁶+12 (c, 1.132 in CHCl₃)

Sigma: P9397

>>Derivative: Di-Ac

CAS Registry Number: 6170-22-5

Molecular Formula: C₂₅H₄₀O₄

Molecular Weight: 404.589

Accurate Mass: 404.29266

Percentage Composition: C 74.22%; H 9.96%; O 15.82%

Melting Point: Mp 135-140°. Mp 152.4° (double Mp)

Optical Rotation: [α]_D²⁶+40.5 (c, 0.778 in CHCl₃)

>>Variant: (3 α ,5 α ,20*S*)-form

CAS Registry Number: 566-58-5

Molecular Formula: C₂₁H₃₆O₂

Molecular Weight: 320.514

Accurate Mass: 320.27153

Percentage Composition: C 78.70%; H 11.32%; O 9.98%

Source/Synthesis: Progesterone metab. isol. from pregnancy urine

Physical Description: Cryst. (EtOH)

Melting Point: Mp 248°

Optical Rotation: [α]_D²⁰+17 (c, 0.15 in EtOH)

Aldrich: 28700-8

Sigma: P9015

>>Derivative: 3-Ac

Molecular Formula: C₂₃H₃₈O₃

Molecular Weight: 362.551

Accurate Mass: 362.282095

Percentage Composition: C 76.20%; H 10.56%; O 13.24%

Physical Description: Plates (MeOH)

Melting Point: Mp 172.5-173.5°

>>Derivative: 20-Ac

Molecular Formula: C₂₃H₃₈O₃

Molecular Weight: 362.551

Accurate Mass: 362.282095

Percentage Composition: C 76.20%; H 10.56%; O 13.24%

Physical Description: Needles (Me₂CO)

Melting Point: Mp 192.5-194°