



CAS Registry Number: 6003-18-5
Molecular Formula: C₂₅H₄₀O₄
Molecular Weight: 404.589
Percentage Composition: C 74.22%; H 9.96%; O 15.82%
Melting Point: Mp 142°
Optical Rotation: $[\alpha]_{\text{D}}^{20} +18$ (c, 0.41 in C₆H₆)
Sigma: P0273

>>Variant: (3 α ,5 β ,20*R*)-form

CAS Registry Number: 80-91-1
Molecular Formula: C₂₁H₃₆O₂
Molecular Weight: 320.514
Accurate Mass: 320.27153
Percentage Composition: C 78.70%; H 11.32%; O 9.98%
Physical Description: Cryst. (EtOH)
Melting Point: Mp 234-235°
Optical Rotation: $[\alpha]_{\text{D}}^{20} +10$

Sigma: P6879

>>Derivative: 3-Ac

CAS Registry Number: 1900-68-1
Molecular Formula: C₂₃H₃₈O₃
Molecular Weight: 362.551
Accurate Mass: 362.282095
Percentage Composition: C 76.20%; H 10.56%; O 13.24%
Physical Description: Cryst. (Me₂CO)
Melting Point: Mp 137-140°

>>Derivative: Di-Ac

CAS Registry Number: 6100-28-3
Molecular Formula: C₂₅H₄₀O₄
Molecular Weight: 404.589
Accurate Mass: 404.29266
Percentage Composition: C 74.22%; H 9.96%; O 15.82%
Physical Description: Cryst. (MeOH)
Melting Point: Mp 112-113°
Optical Rotation: $[\alpha]_{\text{D}}^{26} +61$

>>Variant: (3 α ,5 β ,20*S*)-form

Synonym(s): Pregnanediol

CAS Registry Number: 80-92-2

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. (Me₂CO)
Melting Point: Mp 243-244°
Optical Rotation: $[\alpha]_{\text{D}}^{20} +27.4$ (c, 0.7 in EtOH)

Aldrich: 23461-3
Fluka: 81570
Sigma: P6379