



CAS Registry Number: 95826-69-0
Molecular Formula: C₂₅H₃₈O₇
Molecular Weight: 450.571
Accurate Mass: 450.261755
Percentage Composition: C 66.64%; H 8.50%; O 24.86%
Physical Description: Leaflets (Me₂CO/Et₂O)
Melting Point: Mp 182-183°
Optical Rotation: [α]_D²²+69 (c, 1.5 in CHCl₃)

>>Variant: (3 α ,5 β ,20*S*)-form

Synonym(s): α -Cortolone

CAS Registry Number: 516-42-7

Molecular Formula: C₂₁H₃₄O₅
Molecular Weight: 366.497
Accurate Mass: 366.240625
Percentage Composition: C 68.82%; H 9.35%; O 21.83%
Biological Source: Constit. of human urine
Physical Description: Cryst. (MeOH/EtOAc)
Melting Point: Mp 208-210°
Optical Rotation: [α]_D +44 (EtOH)
Sigma: C5381

>>Derivative: 20,21-Di-Ac

CAS Registry Number: 95826-64-5
Physical Description: Needles (Me₂CO aq.)
Melting Point: Mp 200-201°
Optical Rotation: [α]_D²³+6 (c, 0.56 in CHCl₃)

>>Derivative: 3,20,21-Tri-Ac

Melting Point: Mp 216-217°
Optical Rotation: [α]_D²⁴+28.5 (c, 0.5 in dioxan)

>>Variant: (3 β ,5 α ,20*R*)-form

Molecular Formula: C₂₁H₃₄O₅
Molecular Weight: 366.497
Accurate Mass: 366.240625
Percentage Composition: C 68.82%; H 9.35%; O 21.83%
Melting Point: Mp 177-180°

>>Derivative: 3,20,21-Tri-Ac

Melting Point: Mp 205-206°

>>Variant: (3 β ,5 α ,20*S*)-form

Molecular Formula: C₂₁H₃₄O₅
Molecular Weight: 366.497
Accurate Mass: 366.240625
Percentage Composition: C 68.82%; H 9.35%; O 21.83%

>>Derivative: 20,21-Di-Ac

Physical Description: Cryst. (CHCl₃/MeOH)
Melting Point: Mp 280-282°
Optical Rotation: [α]_D²⁶+5.2 (CHCl₃)

References: