



CAS Registry Number: 16109-53-8
Molecular Formula: C₂₃H₃₆O₅
Molecular Weight: 392.534
Accurate Mass: 392.256275
Percentage Composition: C 70.38%; H 9.24%; O 20.38%
Physical Description: Needles (Me₂CO)
Melting Point: Mp 196-197.5°
Optical Rotation: [α]_D²⁶+87.2 (c, 1 in MeOH)

>>Derivative: 21-Ac

CAS Registry Number: 16065-01-3
Physical Description: Needles (EtOAc)
Melting Point: Mp 229-232°
Optical Rotation: [α]_D²⁶+78.5 (c, 1 in MeOH)

>>Derivative: 3,21-Di-Ac

CAS Registry Number: 16065-02-4
Physical Description: Plates (Me₂CO)
Melting Point: Mp 206-208°
Optical Rotation: [α]_D²⁶+88 (c, 1 in EtOH)

>>Derivative: 21-Ac, 3-O- β -D-glucopyranosiduronic acid

Melting Point: Mp 165-167° (as 2',3',4'-Tri-Ac, Me ester)

>>Variant: (3 β ,5 α ,17 α OH)-form
Synonym(s): Reichstein's Substance P

CAS Registry Number: 516-47-2

Molecular Formula: C₂₁H₃₄O₄
Molecular Weight: 350.497
Accurate Mass: 350.24571
Percentage Composition: C 71.96%; H 9.78%; O 18.26%
Biological Source: Present in adrenals
Physical Description: Needles (EtOH)
Melting Point: Mp 236-239° (210-213°)
Optical Rotation: [α]_D²⁰+48.5 (EtOH)

Sigma: P0768

>>Derivative: 3-Ac

CAS Registry Number: 35458-60-7
Physical Description: Prisms (MeOH/Et₂O)
Melting Point: Mp 195-197°
Optical Rotation: [α]_D¹⁹-42.9 (c, 0.653 in Me₂CO)

>>Derivative: 21-Ac

CAS Registry Number: 63342-00-7
Melting Point: Mp 234-236°
Optical Rotation: [α]_D²⁸+48 (dioxan)

>>Derivative: 3,21-Di-Ac

CAS Registry Number: 6003-22-1
Melting Point: Mp 160-162°
Optical Rotation: [α]_D¹⁹-55.7 (c, 1.633 in Me₂CO)