



>>Derivative: 3,20-Di-Ac

CAS Registry Number: 6170-18-9

Physical Description: Prisms (MeOH)

Melting Point: Mp 159.5-160.5°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +24$ (Me₂CO)

>>Variant: (3β,5α,17αOH,20S)-form

Synonym(s): Reichstein's Substance O

CAS Registry Number: 570-50-3

Molecular Formula: C₂₁H₃₆O₃

Molecular Weight: 336.514

Accurate Mass: 336.266445

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Biological Source: Isol. from adrenal cortex

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 225-227°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -12.55$ (MeOH)

>>Derivative: 3-Ac

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 190-191.5°

Optical Rotation: $[\alpha]_{\text{D}}^{28} -28.6$ (CHCl₃)

>>Derivative: 3,20-Di-Ac

CAS Registry Number: 1176-49-4

Melting Point: Mp 245-247°

Optical Rotation: $[\alpha]_{\text{D}}^{23} -32$ (c, 1 in CHCl₃)

>>Variant: (3β,5α,17βOH,20R)-form

Molecular Formula: C₂₁H₃₆O₃

Molecular Weight: 336.514

Accurate Mass: 336.266445

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Physical Description: Prisms (Me₂CO)

Melting Point: Mp 213-215°

Optical Rotation: $[\alpha]_{\text{D}}^{17} -5.2$ (c, 0.579 in EtOH)

>>Derivative: 3,20-Di-Ac

Physical Description: Platelets (Et₂O/petrol)

Melting Point: Mp 180-0 and 183-185°° (double Mp)

Optical Rotation: $[\alpha]_{\text{D}}^{17} -15.9$ (c, 1.070 in Me₂CO)

>>Variant: (3β,5α,17βOH,20S)-form

Molecular Formula: C₂₁H₃₆O₃

Molecular Weight: 336.514

Accurate Mass: 336.266445

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Physical Description: Leaflets (Et₂O/petrol)

Melting Point: Mp 186-191 and 202-204°° (double Mp)

Optical Rotation: $[\alpha]_{\text{D}}^{18} 0$ (c, 0.510 in Me₂CO)

>>Derivative: 3,20-Di-Ac

Melting Point: Mp 235°

Optical Rotation: $[\alpha]_{\text{D}} -9$ (EtOH)

References: