



>>Entry Name: 17,21-Dihydroxypregn-4-ene-3,20-dione

Related CAS Registry Numbers(s): 601-05-8 1807-15-4 19357-45-0

Type of Compound Code(s): AJ0450 XA1700 XA4300

Structure by analogy with 11,17-Dihydroxypregna-1,4-diene-3,20-dione, [HHL84-Y](#)

Molecular Formula: C₂₁H₃₀O₄

Molecular Weight: 346.466

Accurate Mass: 346.21441

Percentage Composition: C 72.80%; H 8.73%; O 18.47%

Calculated Log P Data: Log P 2.62 (uncertain value) (calc)

>>Variant: 17 α OH-form

Synonym(s): Cortodoxone, BAN, INN, USAN. 17-Hydroxy-11-deoxycorticosterone. 17 α ,21-Dihydroxyprogesterone. Cortexolone. Reichstein's Substance S. NSC 18317. SKF 3050. 11-Deoxycortisol. Cortifen

CAS Registry Number: 152-58-9

Type of Compound Code(s): AJ0450 AJ2800 AJ2650 VT0450

Molecular Formula: C₂₁H₃₀O₄

Molecular Weight: 346.466

Accurate Mass: 346.21441

Percentage Composition: C 72.80%; H 8.73%; O 18.47%

Biological Source: Found in the blood and urine of humans and other mammals

Use/Importance: Glucocorticoid. Antiinflammatory drug

Physical Description: Plates (Et₂O)

Development Status: Never marketed

Melting Point: Mp 207-208°. Mp 212.8-216.8°

Aldrich: 11964-4

Sigma: R0500

>>Derivative: 21-Ac

CAS Registry Number: 640-87-9

Molecular Formula: C₂₃H₃₂O₅

Molecular Weight: 388.503

Accurate Mass: 388.224975

Percentage Composition: C 71.11%; H 8.30%; O 20.59%

Physical Description: Needles (Me₂CO)

Melting Point: Mp 237.2-240.2°

Optical Rotation: [α]_D +114 (116) (Me₂CO)

Sigma: R0625

>>Derivative: 17,21-Acetonide

CAS Registry Number: 85531-15-3

Molecular Formula: C₂₄H₃₄O₄

Molecular Weight: 386.53

Accurate Mass: 386.24571

Percentage Composition: C 74.58%; H 8.87%; O 16.56%

Physical Description: Cryst. (Me₂CO/diisopropyl ether)

Melting Point: Mp 196-202°

Optical Rotation: [α]_D²²+107.4 (c, 1 in CHCl₃)

>>Variant: (9 β ,10 α)-form

Type of Compound Code(s): AJ0450

Molecular Formula: C₂₁H₃₀O₄

Molecular Weight: 346.466

Accurate Mass: 346.21441

Percentage Composition: C 72.80%; H 8.73%; O 18.47%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 225° (dec.)

Optical Rotation: [α]_D²⁵-108 (CHCl₃)

>>Derivative: 21-Ac

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 255-260°

Optical Rotation: [α]