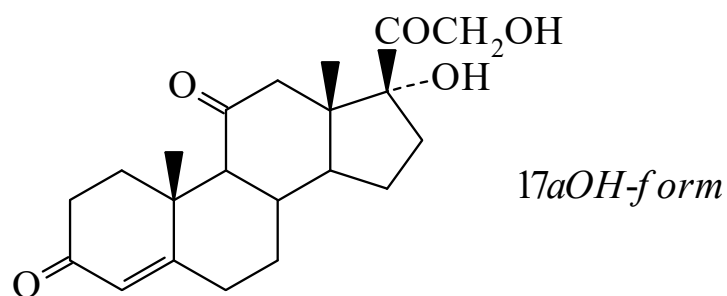




>>Entry Name: 17,21-Dihydroxypregn-4-ene-3,11,20-trione, 9Cl



Type of Compound Code(s): AJ0450

Molecular Formula: C₂₁H₂₈O₅

Molecular Weight: 360.449

Accurate Mass: 360.193675

Percentage Composition: C 69.98%; H 7.83%; O 22.19%

>>Variant: (17αOH)-form

Synonym(s): Cortisone, BAN, INN. 17-Hydroxy-11-dehydrocorticosterone. Kendall's compound E. Reichstein's Substance Fa. Wintersteiner's compound F. NSC 9703. Many other names

CAS Registry Number: 53-06-5

Type of Compound Code(s): XA4300 XA1700 VT0450 AJ0450 AJ2650 AJ2800

Molecular Formula: C₂₁H₂₈O₅

Molecular Weight: 360.449

Accurate Mass: 360.193675

Percentage Composition: C 69.98%; H 7.83%; O 22.19%

Biological Source: Adrenal cortical hormone

Use/Importance: Used in rheumatoid arthritis and rheumatic fever therapy. Glucocorticoid, antiinflammatory agent

Physical Description: Rhombohedral platelets (EtOH)

Melting Point: Mp 220-224°. Mp 230-231°

Optical Rotation: [α]_D +209 (CHCl₃)

Calculated Log P Data: Log P 0.14 (uncertain value) (calc)

Hazard & Toxicity: Adverse effects reported when used therapeutically. Human and exp. teratogen. Exp. reprod. effects

Aldrich: 28543-9

Fluka: 27860

Sigma: C3005

>>Derivative: 21-Me ether

Synonym(s): 17-Hydroxy-21-methoxypregn-4-ene-3,11,20-trione

Type of Compound Code(s): AJ0450

Molecular Formula: C₂₂H₃₀O₅

Molecular Weight: 374.476

Accurate Mass: 374.209325

Percentage Composition: C 70.56%; H 8.07%; O 21.36%

Physical Description: Rosettes (MeOH)

Melting Point: Mp 235-240 dec.°

>>Derivative: 21-Ac

Synonym(s): Cortisone acetate, USAN. Adreson. Many other names

CAS Registry Number: 50-04-4

Type of Compound Code(s): AJ2650 XA4300 XA1700 AJ2800 AJ0450

Molecular Formula: C₂₃H₃₀O₆

Molecular Weight: 402.486

Accurate Mass: 402.20424

Percentage Composition: C 68.64%; H 7.51%; O 23.85%

Use/Importance: Antiinflammatory agent

Physical Description: Needles (Me₂CO)

Melting Point: Mp 239-241°. Mp 243-245°