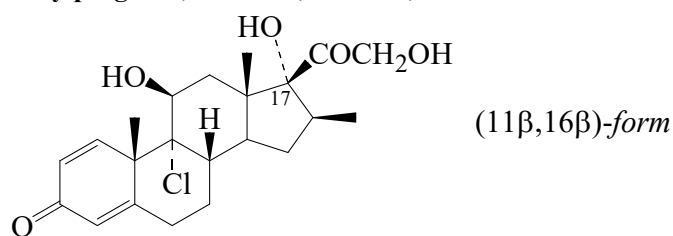




>>Entry Name: 9-Chloro-11,17,21-trihydroxy-16-methylpregna-1,4-diene-3,20-dione, 9Cl



Molecular Formula: C₂₂H₂₉ClO₅

Molecular Weight: 408.921

Accurate Mass: 408.170352

Percentage Composition: C 64.62%; H 7.15%; Cl 8.67%; O 19.56%

Biological Use/Importance: Corticosteroid

Aldrich: 28521-8

Sigma: B0385

>>Variant: (11β,16α)-form

Synonym(s): Icometasone. Icomethasone

CAS Registry Number: 4647-20-5

Molecular Formula: C₂₂H₂₉ClO₅

Molecular Weight: 408.921

Accurate Mass: 408.170352

Percentage Composition: C 64.62%; H 7.15%; Cl 8.67%; O 19.56%

Biological Use/Importance: Corticosteroid

>>Derivative: Formate

Melting Point: Mp 229-234°

Optical Rotation: [α]_D +123 (Py)

>>Derivative: 17-Butanoyl, 21-Ac

Synonym(s): Icomethasone enbutate. CL 09

CAS Registry Number: 103466-73-5

Molecular Formula: C₂₈H₃₇ClO₇

Molecular Weight: 521.049

Accurate Mass: 520.222782

Percentage Composition: C 64.54%; H 7.16%; Cl 6.80%; O 21.49%

Biological Use/Importance: Corticosteroid

>>Variant: (11β,16β)-form

Synonym(s): Beclometasone, INN. Beclomethasone, BAN

CAS Registry Number: 4419-39-0

Molecular Formula: C₂₂H₂₉ClO₅

Molecular Weight: 408.921

Accurate Mass: 408.170352

Percentage Composition: C 64.62%; H 7.15%; Cl 8.67%; O 19.56%

Calculated Log P Data: Log P 1.83 (uncertain value) (calc)

>>Derivative: 21-Ac, 17-pentanoyl

Synonym(s): Beclometasone valeroacetate

CAS Registry Number: 57780-94-6

Molecular Formula: C₂₉H₃₉ClO₇

Molecular Weight: 535.076

Accurate Mass: 534.238432

Percentage Composition: C 65.10%; H 7.35%; Cl 6.63%; O 20.93%

Biological Use/Importance: Glucocorticoid. Topical antiinflammatory agent

Melting Point: Mp 117-119°

Optical Rotation: [α]_D +94 (c, 0.96 in CHCl₃)

Calculated Log P Data: Log P 4.49 (uncertain value) (calc)