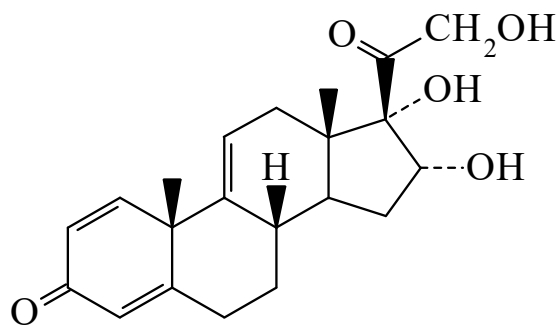




>>Entry Name: 16,17,21-Trihydroxypregna-1,4,9(11)-triene-3,20-dione, 9Cl



Molecular Formula: C₂₁H₂₆O₅

Molecular Weight: 358.433

Accurate Mass: 358.178025

Percentage Composition: C 70.37%; H 7.31%; O 22.32%

>>Variant: (16 α ,17 α OH)-form

CAS Registry Number: 39672-76-9

Molecular Formula: C₂₁H₂₆O₅

Molecular Weight: 358.433

Accurate Mass: 358.178025

Percentage Composition: C 70.37%; H 7.31%; O 22.32%

Source/Synthesis: Obt. by incubation of 3 β ,21-diacetoxy-16 α ,17-dihydroxy-5 α -pregn-9(11)-en-20-one with *Bacterium havaniensis*

Physical Description: Cryst. (Me₂CO/petrol)

Optical Rotation: [α]_D²²+8.6 (c, 1 in CHCl₃)

>>Derivative: 21-Ac

CAS Registry Number: 77017-20-0

Molecular Formula: C₂₃H₂₈O₆

Molecular Weight: 400.471

Accurate Mass: 400.18859

Percentage Composition: C 68.98%; H 7.05%; O 23.97%

Physical Description: Cryst. (Me₂CO/petrol)

Melting Point: Mp 213-215°

Optical Rotation: [α]_D²⁵+3.9 (c, 1 in MeOH)

>>Derivative: 16,21-Di-Ac

Molecular Formula: C₂₅H₃₀O₇

Molecular Weight: 442.508

Accurate Mass: 442.199155

Percentage Composition: C 67.86%; H 6.83%; O 25.31%

Physical Description: Needles (Me₂CO/petrol)

Melting Point: Mp 200-201°

Optical Rotation: [α]_D²⁵-2.9 (c, 1 in MeOH)

References:

U.S. Pat., 1962, 3 047 468; *CA*, **58**, 568, (*synth*)