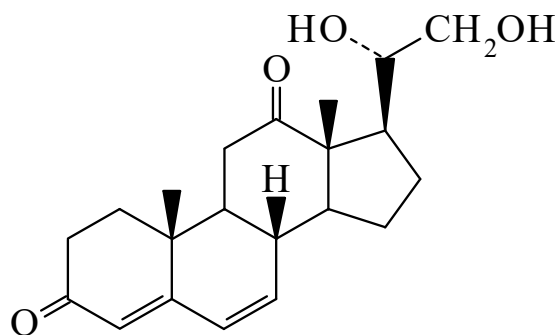




>>Entry Name: 20,21-Dihydroxypregna-4,6-diene-3,12-dione, 9Cl



Type of Compound Code(s): AJ0450 VT0450

Molecular Formula: C₂₁H₂₈O₄

Molecular Weight: 344.45

Accurate Mass: 344.19876

Percentage Composition: C 73.23%; H 8.19%; O 18.58%

>>Variant: (20S)-form

Synonym(s): Neridienone B

CAS Registry Number: 61671-56-5

Type of Compound Code(s): VT0450 AJ0450

Molecular Formula: C₂₁H₂₈O₄

Molecular Weight: 344.45

Accurate Mass: 344.19876

Percentage Composition: C 73.23%; H 8.19%; O 18.58%

Biological Source: Constit. of *Nerium odorum*

Physical Description: Cryst. (Me₂CO/hexane)

Melting Point: Mp 179-181°

Optical Rotation: [α]_D +85.7 (c, 1.2 in CHCl₃)

>>Derivative: 21-Ac

CAS Registry Number: 61671-10-1

Molecular Formula: C₂₃H₃₀O₅

Molecular Weight: 386.487

Accurate Mass: 386.209325

Percentage Composition: C 71.48%; H 7.82%; O 20.70%

Melting Point: Mp 173-175°

Optical Rotation: [α]_D²⁰ +59.8 (c, 0.64 in CHCl₃)

>>Derivative: Di-Ac

CAS Registry Number: 61671-11-2

Molecular Formula: C₂₅H₃₂O₆

Molecular Weight: 428.524

Accurate Mass: 428.21989

Percentage Composition: C 70.07%; H 7.53%; O 22.40%

Physical Description: Solid

Optical Rotation: [α]_D²⁰ +78.6 (c, 3.44 in CHCl₃)

References:

Abe, F. *et al.*, *Phytochemistry*, 1976, **15**, 1745, (*isol*)