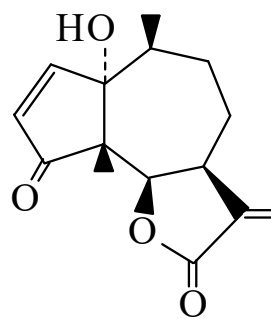




>>Entry Name: 1-Hydroxy-4-oxo-2,11(13)-pseudoguaiadien-12,6-olide



Molecular Formula: C₁₅H₁₈O₄

Molecular Weight: 262.305

Accurate Mass: 262.12051

Percentage Composition: C 68.69%; H 6.92%; O 24.40%

Use/Importance: Adrenoceptor blocking agent. Antineoplastic agent, CNS depressant. Possesses antimalarial and antiauxin activity

Calculated Log P Data: Log P 0.13 (calc)

>>Variant: (1 α ,5 β ,6 β ,10 β)-form

Synonym(s): Parthenin

CAS Registry Number: 508-59-8

Molecular Formula: C₁₅H₁₈O₄

Molecular Weight: 262.305

Accurate Mass: 262.12051

Percentage Composition: C 68.69%; H 6.92%; O 24.40%

Biological Source: Bitter principle of *Parthenium hysterophorus* and *Iva nevadensis*

Physical Description: Cryst. (H₂O)

Melting Point: Mp 163-166°

Optical Rotation: [α]_D²⁵+7.02 (c, 2.71 in CHCl₃)

Solubility: BERDY SOL: Sol. MeOH, CHCl₃; poorly sol. H₂O

UV: [neutral] $\lambda_{\max}$ 215 (ϵ 13100); 340 (ϵ 20) (MeOH) (Berdy)

Other Data: Pharmacol. active isomer

Hazard & Toxicity: Can cause contact dermatitis. LD₅₀ (rat, ipr) 42 mg/kg

>>Derivative: 11,13-Dihydro

Synonym(s): 1-Hydroxy-4-oxo-2-pseudoguaien-12,6-olide. Dihydroparthenin

Molecular Formula: C₁₅H₂₀O₄

Molecular Weight: 264.321

Accurate Mass: 264.13616

Percentage Composition: C 68.16%; H 7.63%; O 24.21%

Biological Source: Constit. of *Parthenium hysterophorus*

Physical Description: Cryst.

Melting Point: Mp 145°

>>Derivative: 1,2-Dihydro

Synonym(s): 1-Hydroxy-4-oxo-11(13)-pseudoguaien-12,6-olide. Coronopilin. 1,2-Dihydroparthenin

CAS Registry Number: 2571-81-5

Molecular Formula: C₁₅H₂₀O₄

Molecular Weight: 264.321

Accurate Mass: 264.13616

Percentage Composition: C 68.16%; H 7.63%; O 24.21%

Biological Source: Constit. of *Parthenium incanum*, *Ambrosia psilostachya*, *Ambrosia artemisiifolia*, *Iva nevadensis* and *Iva acerosa*

Use/Importance: Antineoplastic agent

Physical Description: Cryst. (Me₂CO/diisopropyl ether)

Melting Point: Mp 177-178°

Optical Rotation: [α]_D²¹-30.2 (c, 4.2 in EtOH)

Calculated Log P Data: Log P 0.52 (calc)

UV: [neutral] $\lambda_{\max}$ 213 (ϵ 9800); 290 (ϵ 29) (EtOH) (Berdy)