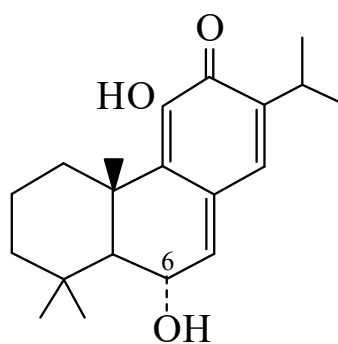




>>Entry Name: 6,11-Dihydroxy-7,9(11),13-abietatrien-12-one



Molecular Formula: C₂₀H₂₈O₃

Molecular Weight: 316.439

Accurate Mass: 316.203845

Percentage Composition: C 75.91%; H 8.92%; O 15.17%

>>Variant: 6 α -form

Synonym(s): Taxodone. NSC 122420

CAS Registry Number: 19039-02-2

Molecular Formula: C₂₀H₂₈O₃

Molecular Weight: 316.439

Accurate Mass: 316.203845

Percentage Composition: C 75.91%; H 8.92%; O 15.17%

Biological Source: Isol. from *Taxodium distichum*

Use/Importance: Shows antineoplastic activity

Physical Description: Yellow plates (Et₂O/petrol)

Melting Point: Mp 164-165°

Optical Rotation: [α]_D²⁵+50 (c, 2.5 in CHCl₃)

Solubility: BERDY SOL: Sol. MeOH, Et₂O; poorly sol. H₂O, hexane

Calculated Log P Data: Log P 4.03 (calc)

UV: [acid] $\lambda_{\max}$ (no solvent specified) (Derep) [neutral] $\lambda_{\max}$ 316 (ϵ 20000) (MeOH) (Derep) [neutral] $\lambda_{\max}$ 316 (ϵ 20000) (MeOH) (Berdy)

>>Derivative: 6-Ketone

Synonym(s): 11-Hydroxy-7,9(11),13-abietatriene-6,12-dione. **Taxodione.** NSC 122419

CAS Registry Number: 19026-31-4

Molecular Formula: C₂₀H₂₆O₃

Molecular Weight: 314.424

Accurate Mass: 314.188195

Percentage Composition: C 76.40%; H 8.33%; O 15.27%

Biological Source: Isol. from *Taxodium distichum*

Use/Importance: Shows antineoplastic activity

Physical Description: Golden plates (MeOH)

Melting Point: Mp 115-116°

Optical Rotation: [α]_D²⁵+56 (c, 1 in CHCl₃)

Solubility: BERDY SOL: Sol. MeOH, Et₂O; poorly sol. H₂O, hexane

Calculated Log P Data: Log P 3.78 (calc)

UV: [base] $\lambda_{\max}$ 265 (ϵ); 295 (ϵ); 485 (ϵ) (MeOH/NH₃) (Derep) [neutral] $\lambda_{\max}$ 320 (ϵ 25000); 332 (ϵ 26000); 400 (ϵ 2000) (MeOH) (Derep) [neutral] $\lambda_{\max}$ 224 (ϵ 10471); 320 (ϵ 25000); 324 (ϵ 19500); 332 (ϵ 26000); 333 (ϵ 19950); 400 (ϵ 2000); 405 (ϵ 251) (MeOH) (Berdy)

References:

- Kupchan, S.M. *et al.*, *J.O.C.*, 1969, **34**, 3912, (*isol, struct*)
Matsumoto, T. *et al.*, *Bull. Chem. Soc. Jpn.*, 1977, **50**, 1575, (*synth*)
Johnson, W.S. *et al.*, *Tetrahedron*, 1982, **38**, 1397, (*synth*)
Burnell, R.H. *et al.*, *Can. J. Chem.*, 1987, **65**, 775, (*synth*)
Haslinger, E. *et al.*, *Annalen*, 1989, 677, (*synth*)
Sánchez, A.J. *et al.*, *J.O.C.*, 1994, **59**, 5445, (*synth*)
Harring, S.R. *et al.*, *Tetrahedron*, 1994, **50**, 9229, (*synth*)