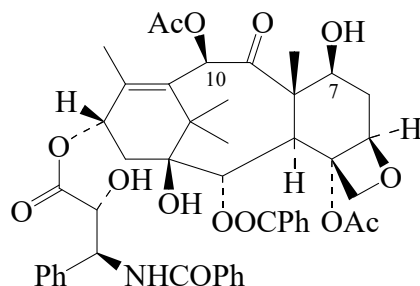




>>>Entry Name: TaxolTM

Synonym(s): Paclitaxel, BAN, INN, USAN. Taxol A. Anzatax. Yewtaxan. BMS 181339-01. NSC 125973



CAS Registry Number: 33069-62-4

Molecular Formula: C₄₇H₅₁NO₁₄

Molecular Weight: 853.918

Accurate Mass: 853.330959

Percentage Composition: C 66.11%; H 6.02%; N 1.64%; O 26.23%

5,20-Epoxy-11-taxene-1,2,4,7,9,10,13-heptol JNV64-C). Also reported in traces from the fungus *Taxomyces andreanae*

Biological Use/Importance: Antileukaemic and antineoplastic agent, esp. against melanoma and ovarian tumours. Use limited by low solubility and scarce availability of *Taxus brevifolia* bark. Biochemical tool extensively used to study cellular shape and function. Also shown to be active against oomycete fungi

Physical Description: Needles (MeOH aq.)

Development Status: Marketed drug. Launched 1993 (US, Canada, Sweden). Worldwide 24th best selling prescription drug (\$1.59 bn) (Bristol-Myers Squibb) (2000, Pharma Business)

Melting Point: Mp 213-216°

Optical Rotation: $[\alpha]_D^{20}$ -49 (MeOH)

Calculated Log P Data: Log P 2.47 (uncertain value) (calc)

UV: [neutral] $\lambda_{\max}$ 227 (ϵ 29800); 273 (ϵ 1700) (MeOH) (Derep) [neutral] $\lambda_{\max}$ 230 (); 280 () (MeOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, ipr) 128 mg/kg. LD₅₀ (mus, ivn) 12 mg/kg

Aldrich: 41701-7

Fluka: 86346

Sigma: T7402

Other: CarboMer Inc. (3 grades)

>>>Derivative: 7-O- β -D-Xylopyranoside

Synonym(s): 7-Xylosyltaxol

CAS Registry Number: 90332-66-4

Molecular Formula: C₅₂H₅₉NO₁₈

Molecular Weight: 986.034

Accurate Mass: 985.373219

Percentage Composition: C 63.34%; H 6.03%; N 1.42%; O 29.21%

Biological Source: Constit. of *Taxus baccata*

Physical Description: Cryst. (2-propanol)

Melting Point: Mp 236-238°

Optical Rotation: $[\alpha]_D$ -23 (Py)

UV: [neutral] $\lambda_{\max}$ 227 (ϵ 29800); 273 (ϵ 1700) (MeOH) (Derep)

>>>Derivative: 2',7-Di-Ac

Synonym(s): 2',7-Diacetyltaxol

Molecular Formula: C₅₁H₅₅NO₁₆

Molecular Weight: 937.993

Accurate Mass: 937.352089

Percentage Composition: C 65.31%; H 5.91%; N 1.49%; O 27.29%

Biological Source: Constit. of *Taxus brevifolia*

Physical Description: Needles

Melting Point: Mp 227-228°

Solubility: Poorly sol. hexane