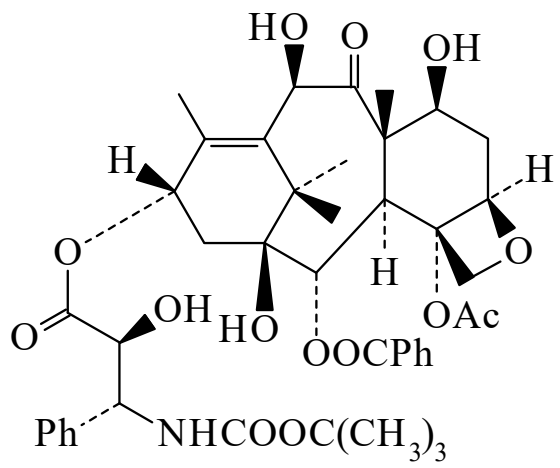
>>**Entry Name: Docetaxel,** BAN, INN
Synonym(s): *N*-Debenzoyl-*N*-*tert*-butoxycarbonyl-10-deacetyltaxol. Taxotere. NSC 628503



CAS Registry Number: 114977-28-5
Related CAS Registry Numbers(s): 148408-66-6
Type of Compound Code(s): XA1950

Molecular Formula: $C_{43}H_{53}NO_{14}$
Molecular Weight: 807.89
Accurate Mass: 807.346609
Percentage Composition: C 63.93%; H 6.61%; N 1.73%; O 27.73%
Source/Synthesis: Synth. from baccatin III (see 5,20-Epoxy-11-taxene-1,2,4,7,9,10,13-heptol JNV64-C)
Biological Use/Importance: Antineoplastic agent. Antimicrotubule agent. Under investigation for treatment of ovarian, breast and bronchial carcinomas
Physical Description: Cryst. (MeOH)
Development Status: Marketed drug. Launched 1995 (South Africa). Worldwide 73rd best selling prescription drug ($0.69 bn) (Aventis) (2000, Pharma Business)
Melting Point: Mp 232°
Optical Rotation: $[\alpha]_D$ –36 (c, 0.74 in EtOH)
Calculated Log P Data: Log P 1.97 (uncertain value) (calc)

>>**Derivative:** Ac

CAS Registry Number: 125354-16-7
Molecular Formula: $C_{45}H_{55}NO_{15}$
Molecular Weight: 849.927
Percentage Composition: C 63.59%; H 6.52%; N 1.65%; O 28.24%
Physical Description: Cryst. (MeOH)
Melting Point: Mp 201-203°

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