



Synonym(s): 2-Debenzoyl-2-tigloyl-10-deacetylbaccatin III

Molecular Formula: C₂₇H₃₈O₁₀

Molecular Weight: 522.591

Accurate Mass: 522.2465

Percentage Composition: C 62.06%; H 7.33%; O 30.62%

Biological Source: Constit. of *Taxus baccata*

Physical Description: Amorph.

Optical Rotation: [α]_D²⁵ -30.4 (c, 0.5 in EtOH)

UV: [neutral] $\lambda_{\max}$ 218 () (MeOH) (Berdy)

>>**Derivative:** 9-Ketone, 2-benzoyl, 4-Ac

Synonym(s): 10-Deacetylbaccatin III

CAS Registry Number: 32981-86-5

Molecular Formula: C₂₉H₃₆O₁₀

Molecular Weight: 544.597

Accurate Mass: 544.23085

Percentage Composition: C 63.96%; H 6.66%; O 29.38%

Biological Source: Found in leaves and twigs of *Taxus baccata*; also obt. from [LFR07-L](#) by mild hydrol.

Use/Importance: Intermed. in coml. synthesis of TaxolTM [JNQ02-J](#) from the readily available *T. baccata* (Bristol-Myers Squibb, 1993). Also an intermed. for the semisynthetic drug Docetaxel [LRX16-X](#)

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

UV: [neutral] $\lambda_{\max}$ 254 (ϵ 1070); 278 (ϵ 12880) (EtOH) (Berdy)

Other: Janssen, Spectrum Chemical

>>**Derivative:** 9-Ketone, 2-benzoyl, 1,4-di-Ac

Molecular Formula: C₃₁H₃₈O₁₁

Molecular Weight: 586.635

Accurate Mass: 586.241415

Percentage Composition: C 63.47%; H 6.53%; O 30.00%

Biological Source: Constit. of *Taxus canadensis*

>>**Derivative:** 9-Ketone, 2-benzoyl, 4,10-di-Ac

Synonym(s): Baccatin III

CAS Registry Number: 27548-93-2

Molecular Formula: C₃₁H₃₈O₁₁

Molecular Weight: 586.635

Accurate Mass: 586.241415

Percentage Composition: C 63.47%; H 6.53%; O 30.00%

Biological Source: Isol. from *Taxus baccata*

Physical Description: Cryst.

Melting Point: Mp 233-234°

Optical Rotation: [α]_D -93

UV: [neutral] $\lambda_{\max}$ 230 (ϵ 13900); 274 (ϵ 1000); 280 (ϵ 850) (MeOH) (Berdy)

Sigma: B8154

>>**Derivative:** 9-Ketone, 2-benzoyl, 4,10-di-Ac, 7-O- β -D-xylopyranoside

Synonym(s): 7-Xylosylbaccatin III

CAS Registry Number: 203851-94-9

Molecular Formula: C₃₆H₄₆O₁₅

Molecular Weight: 718.75

Accurate Mass: 718.283675

Percentage Composition: C 60.16%; H 6.45%; O 33.39%

Biological Source: Constit. of *Taxus yunnanensis*

Physical Description: Amorph. powder