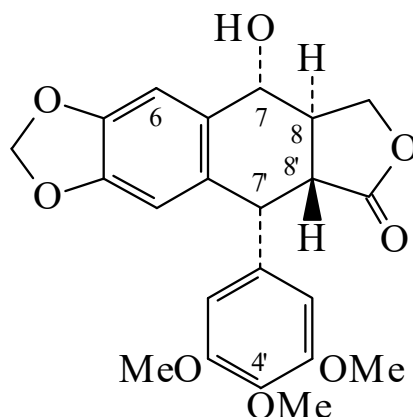




>>Entry Name: Podophyllotoxin, BAN

ENTRY UNDER REVIEW

Synonym(s): 7-Hydroxy-3',4',5'-trimethoxy-4,5-methylenedioxy-2,7'-cyclo lignan-9',9-olide. Podofilox, USAN. Condylina. Condylon. Warticon. NSC 24818



CAS Registry Number: 518-28-5

Related CAS Registry Numbers(s): 77519-37-0

Molecular Formula: C₂₂H₂₂O₈

Molecular Weight: 414.411

Accurate Mass: 414.13147

Percentage Composition: C 63.76%; H 5.35%; O 30.89%

Biological Source: Lignan from *Podophyllum emodi* rhizomes. Also isol. from *Podophyllum peltatum*, other *Podophyllum* spp., *Diphylleia grayi*, *Callitris drummondii*, *Juniperus* spp. and *Linum flavum*

Use/Importance: Potent cytotoxin. Cell division inhibitor; inhibitor of human DNA topoisomerase II. Antimitotic agent. Used topically for treatment of external ano-genital warts and plantar warts

Physical Description: Cryst. (Me₂CO aq. or MeOH)

Melting Point: Mp 117-118°

Optical Rotation: [α]_D¹⁴ -101.3 (EtOH)

Solubility: BERDY SOL: Sol. H₂O

Calculated Log P Data: Log P -0.84 (calc)

UV: [neutral] $\lambda_{\max}$ 289 (ϵ 3500) (EtOH) (Derep) [neutral] $\lambda_{\max}$ 292 () (MeOH) (Berdy) [neutral] $\lambda_{\max}$ 287 (ϵ 4300); 291 (ϵ 4350) (EtOH) (Berdy)

Other Data: 4 Crystal modifications reported. Mp's up to 188-189° have been reported for carefully dried samples

Hazard & Toxicity: Severe eye, skin and respiratory tract irritant. Severe adverse effects reported if swallowed incl. gastrointestinal, CNS, hepatotoxic, nephrotoxic, haemopoietic effects and development of peripheral and autonomic neuropathies. LD₅₀ (rat, skn) 500 mg/kg. LD₅₀ (mus, orl) 100 mg/kg ; BERDY HAZD : LD₅₀ (mus, orl) 90 mg/kg

Aldrich: 85844-7

Fluka: 81125

Rare Chemicals Library: S40567-1

Sigma: P4405

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

Molecular Formula: C₂₈H₃₂O₁₃

Molecular Weight: 576.553

Accurate Mass: 576.184295

Percentage Composition: C 58.33%; H 5.59%; O 36.08%

Biological Source: Isol. from *Podophyllum emodi* and from plants and cell cultures of *Linum flavum*

Use/Importance: Antineoplastic agent

Physical Description: Amorph. solid

Melting Point: Mp 149-152°

Optical Rotation: [α]_D²⁰ -65 (c, 0.5 in H₂O). [α]_D -75 (c, 0.6 in MeOH). [α]_D -117 (c, 0.67 in Py)

Calculated Log P Data: Log P -3.13 (uncertain value) (calc)

>>Derivative: Ac

CAS Registry Number: 1180-34-3

Physical Description: Cryst. (MeOH)

Melting Point: Mp 209.5-210.5°

Optical Rotation: [α]_D²⁰ -143 (c, 1 in CHCl₃)