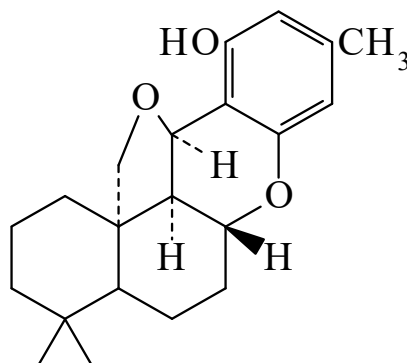




>>Entry Name: Siccanin, INN, JAN

Synonym(s): 1,2,3,4,4a,5,6,6a,11b,13b-Decahydro-4,4,6a,9-tetramethyl-13H-benzo[a]furo[2,3,4-mn]xanthen-11-ol, 9Cl. Tackle. CS 280. SI 23548



CAS Registry Number: 22733-60-4

Molecular Formula: C₂₂H₃₀O₃

Molecular Weight: 342.477

Accurate Mass: 342.219495

Percentage Composition: C 77.16%; H 8.83%; O 14.02%

Biological Source: Isol. from cultures of *Helminthosporium siccans*, a parasitic organism of ryegrass

Use/Importance: Antifungal agent

Physical Description: Cryst.

Melting Point: Mp 139-140°

Optical Rotation: $[\alpha]_D^{20} -136$ (c, 2 in CHCl₃)

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

pKa Value: pK_a 10.9

Calculated Log P Data: Log P 5.7 (uncertain value) (calc)

UV: [neutral] $\lambda_{\max}$ 210 (ϵ 45900); 285 (ϵ 1717) (MeOH) (Berdy) [neutral] $\lambda_{\max}$ 278 (E1%/1cm 92); 285 (E1%/1cm 74) (EtOH) (Berdy)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ipr) 1700 mg/kg

>>Derivative: 4-Bromobenzenesulfonyl

Physical Description: Orthorhombic cryst.

Melting Point: Mp 156°

References:

- Ishibashi, K., *J. Antibiot., Ser. A*, 1962, **15**, 161, (*isol*)
Hirai, K. *et al.*, *Acta Cryst. B*, 1969, **25**, 2630, (*cryst struct*)
Hirai, K. *et al.*, *Tetrahedron*, 1971, **27**, 6057, (*struct, uv, ir, ms, pmr*)
Suzuki, K.T. *et al.*, *Bioorg. Chem.*, 1974, **3**, 72, (*biosynth*)
Bellotti, M.G. *et al.*, *Chemotherapy (Basel)*, 1985, **4**, 431, (*props*)
Kato, M. *et al.*, *Tetrahedron*, 1987, **43**, 711, (*synth*)