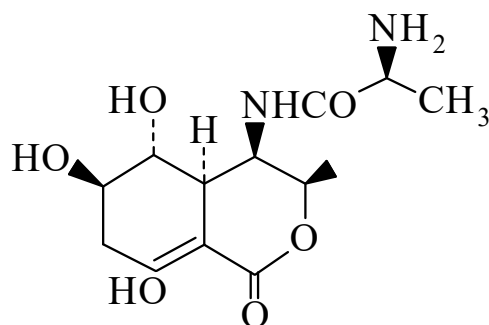




>>Entry Name: Actinobolin

Synonym(s): 2-Amino-*N*-(3,4,4*a*,5,6,7-hexahydro-5,6,8-trihydroxy-3-methyl-1-oxo-1*H*-2-benzopyran-4-yl)propanamide, 9Cl. Actinovorin. NSC 31083



CAS Registry Number: 24397-89-5

Molecular Formula: C₁₃H₂₀N₂O₆

Molecular Weight: 300.311

Accurate Mass: 300.132138

Percentage Composition: C 51.99%; H 6.71%; N 9.33%; O 31.97%

Biological Source: From *Streptomyces griseoviridis* var. *atrofaciens*

Use/Importance: Broad-spectrum antibiotic. Possesses antineoplastic props. Exp. cariostat

Physical Description: Amorph. powder

Optical Rotation: $[\alpha]_D^{28} +59$ (c, 0.5 in pH 7 phosphate buffer)

Solubility: Sol. H₂O, EtOH; BERDY SOL: Sol. H₂O; fairly sol. MeOH, EtOH, butanol; poorly sol. Me₂CO, hexane

pKa Value: pK_{a1} 7.5; pK_{a2} 8.8

Calculated Log P Data: Log P -3.41 (calc)

UV: [acid] $\lambda_{\max}$ 263 (ϵ 19600) (0.1*N* HCl) (Derep) [base] $\lambda_{\max}$ 288 (ϵ 29800) (0.1*N* NaOH) (Derep) [neutral] $\lambda_{\max}$ 264 (ϵ 18600) (pH 7 phosphate buffer) (Derep) [neutral] $\lambda_{\max}$ 264 (E1%/1cm 253) (pH 7 buffer) (Berdy) [acid] $\lambda_{\max}$ 263 (E1%/1cm 266) (HCl) (Berdy) [base] $\lambda_{\max}$ 288 (E1%/1cm 406) (NAOH) (Berdy)

Other Data: Unstable in alk. soln.

Hazard & Toxicity: LD₅₀ (mus, ipr) 2844 mg/kg ; BERDY HAZD : LD₅₀ (mus, ivn) 800 mg/kg

>>Derivative: Sulfate (2:1)

CAS Registry Number: 18802-17-0

Physical Description: Cryst. (EtOH aq.)

Optical Rotation: $[\alpha]_D^{22} +54.5$ (c, 1 in H₂O)

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