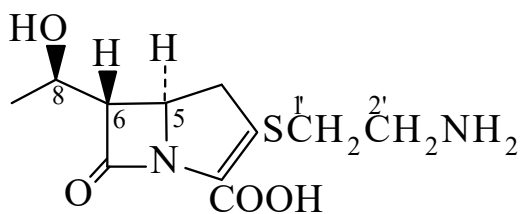




>>Entry Name: Thienamycin



CAS Registry Number: 59995-64-1

Related CAS Registry Numbers(s): 63701-31-5 68399-24-6 68510-61-2 74923-12-9 75657-62-4 77448-04-5

Molecular Formula: C₁₁H₁₆N₂O₄S

Molecular Weight: 272.324

Accurate Mass: 272.083078

Percentage Composition: C 48.52%; H 5.92%; N 10.29%; O 23.50%; S 11.77%

Biological Source: Prod. by *Streptomyces cattleya*

Use/Importance: Active against gram-positive and -negative bacteria

Melting Point: Mp 205 dec.°

Optical Rotation: [α]_D²⁷+82.7 (c, 0.1 in 10mM phosphate buffer, pH 6.95)

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

pKa Value: pK_a 3.08 (30mM phosphate buffer)

UV: [neutral] $\lambda_{\max}$ 297 (E1%/1cm 355) (H₂O) (Berdy) [acid] $\lambda_{\max}$ 309 () (pH 2 buffer) (Berdy) [base] $\lambda_{\max}$ 300 () (pH 12 buffer) (Berdy)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ivn) 3500 mg/kg

>>Derivative: N-Ac

Synonym(s): N-Acetylthienamycin

CAS Registry Number: 63701-32-6

Molecular Formula: C₁₃H₁₈N₂O₅S

Molecular Weight: 314.362

Accurate Mass: 314.093643

Percentage Composition: C 49.67%; H 5.77%; N 8.91%; O 25.45%; S 10.20%

Biological Source: Isol. from *Streptomyces* spp.

Use/Importance: Active against gram-positive and -negative bacteria

UV: [neutral] $\lambda_{\max}$ 301 (E1%/1cm 208) (H₂O) (Berdy)

>>Derivative: N-Formimidoyl

>>Derivative: 1',2'-Didehydro, N-Ac

Synonym(s): N-Acetyldehydrothienamycin

CAS Registry Number: 68738-07-8

Molecular Formula: C₁₃H₁₆N₂O₅S

Molecular Weight: 312.346

Accurate Mass: 312.077993

Percentage Composition: C 49.99%; H 5.16%; N 8.97%; O 25.61%; S 10.27%

Biological Source: From *Streptomyces cattleya*

UV: [neutral] $\lambda_{\max}$ 228 (); 308 () (H₂O) (Berdy)