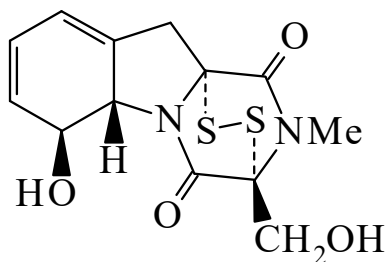




>>Entry Name: Gliotoxin

Synonym(s): 2,3,5a,6-Tetrahydro-6-hydroxy-3-(hydroxymethyl)-2-methyl-10*H*-3,10*a*-epidithiopyrazino[1,2-*a*]indole-1,4-dione, 9Cl, 8Cl. **Aspergillin₊**. SN 12870. Antibiotic SN 12870



CAS Registry Number: 67-99-2

Molecular Formula: C₁₃H₁₄N₂O₄S₂

Molecular Weight: 326.397

Accurate Mass: 326.039498

Percentage Composition: C 47.84%; H 4.32%; N 8.58%; O 19.61%; S 19.65%

Biological Source: Isol. from *Gliocladium fimbriatum*, *Aspergillus fumigatus* and *Penicillium* spp.

Use/Importance: Shows antiviral activity, of limited use as agricultural fungicide. Now superseded. Also shows immunomodulating activity

Physical Description: Monoclinic cryst. (MeOH)

Melting Point: Mp 221 dec.°

Optical Rotation: [α]_D²⁵ -290 (c, 0.078 in EtOH)

Calculated Log P Data: Log P 1.13 (uncertain value) (calc)

UV: [neutral] $\lambda_{\max}$ 269 (ϵ 4500); 310 (ϵ); 340 (ϵ) (MeOH) (Derep)

Hazard & Toxicity: LD₅₀ (mus, orl) 67 mg/kg, hepatotoxic

Fluka: 48975

Sigma: G9893

>>Derivative: Ac

Synonym(s): Acetylgliotoxin

Molecular Formula: C₁₅H₁₆N₂O₅S₂

Molecular Weight: 368.434

Accurate Mass: 368.050063

Percentage Composition: C 48.90%; H 4.38%; N 7.60%; O 21.71%; S 17.41%

Biological Source: Isol. from *Penicillium terlikowskii*

Use/Importance: Antibiotic

Physical Description: Pale-yellow rhombic cryst. (C₆H₆)

Melting Point: Mp 162-163°

Optical Rotation: [α]_D¹⁹ -197 (c, 0.6 in CHCl₃)

Solubility: BERDY SOL: Sol. MeOH, Et₂O; poorly sol. H₂O

UV: [neutral] $\lambda_{\max}$ 0 (end) (ϵ) (MeOH) (Derep) [neutral] $\lambda_{\max}$ 268 (ϵ 6300) (EtOH) (Berdy)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ipr) 50 mg/kg

>>Derivative: Dibenzoyl

Physical Description: Plates (CHCl₃/MeOH)

Melting Point: Mp 192-193 dec.°

Optical Rotation: [α]_D²² -20 (c, 1 in CHCl₃)

>>Derivative: Bis(4-bromobenzoyl)

Physical Description: Needles (dioxan aq.)

Melting Point: Mp 193 dec.°

Optical Rotation: [α]_D -20 (c, 1 in CHCl₃)

>>Derivative: Bis(4-nitrobenzoyl)

Physical Description: Prismatic rods (CHCl₃/MeOH)

Melting Point: Mp 189 dec.°

Optical Rotation: [α]_D²² -13 (c, 1 in CHCl₃)