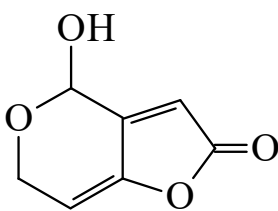




>>Entry Name: Patulin

ENTRY UNDER REVIEW

Synonym(s): 4-Hydroxy-4*H*-furo[3,2-*c*]pyran-2(6*H*)-one, 9Cl, 8Cl. Clavacin. Clavatin. Claviformin. Expansin. Flavicin. **Gigantic acid**†. Mycoin C₃. Penicidin. Terinin. YS 1649. Antibiotic YS 1649. Sch 351633. Antibiotic Sch 351633



CAS Registry Number: 149-29-1

Molecular Formula: C₇H₆O₄

Molecular Weight: 154.122

Accurate Mass: 154.02661

Percentage Composition: C 54.55%; H 3.92%; O 41.52%

Biological Source: Antibiotic produced by several fungi, e.g. *Aspergillus clavatus*, *Aspergillus terreus*, *Penicillium patulum* and *Penicillium griseofulvum*

Use/Importance: Seed germination inhibitor. Shows antibacterial props. Inhibitor of hepatitis C virus protease. Sometimes detd. in apple juice

Physical Description: Prisms or plates (Et₂O or CHCl₃)

Melting Point: Mp 111°

Optical Rotation: [α]_D²¹ -6.2 (CHCl₃)

Calculated Log P Data: Log P -2.4 (uncertain value) (calc)

UV: [acid] λ_{max} (no shifts reported) (Derep) [base] λ_{max} 292 (ε 13400) (0.1*N* NaOH) (Derep) [neutral] λ_{max} 276 (ε 14800) (H₂O or MeOH) (Derep)

Hazard & Toxicity: Exp. neoplastic agent and teratogen. LD₅₀ (rat, orl) 27.8 mg/kg. Exp. kidney and gastrointestinal effects

Aldrich: 85958-3

Sigma: P1639

Supelco: R47-4470

>>Derivative: Phenylhydrazone

Melting Point: Mp 149-150°

>>Derivative: Ac

CAS Registry Number: 6192-26-3

Molecular Formula: C₉H₈O₅

Molecular Weight: 196.159

Accurate Mass: 196.037175

Percentage Composition: C 55.11%; H 4.11%; O 40.78%

Physical Description: Prisms (EtOH aq.)

Melting Point: Mp 118-120°

References: