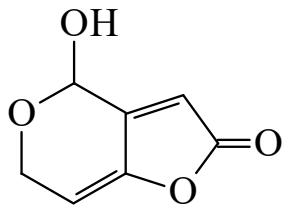
>>**Entry Name: Patulin**

ENTRY UNDER REVIEW

Synonym(s): 4-Hydroxy-4*H*-furo[3,2-*c*]pyran-2(6*H*)-one, 9CI, 8CI. Clavacin. Clavatin. Claviformin. Expansin. Flavicin. **Gigantic acid‡.** Mycoin C_3. Penicidin. Terinin. YS 1649. Antibiotic YS 1649. Sch 351633. Antibiotic Sch 351633



CAS Registry Number: 149-29-1

Molecular Formula: $C_7H_6O_4$
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 hepatitus C virus protease. Sometimes detd. in apple juice
Physical Description: Prisms or plates (Et_2O or $CHCl_3$)
Melting Point: Mp 111°
Optical Rotation: $[\alpha]_D^{21}$ –6.2 ($CHCl_3$)
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) (H_2O or MeOH) (Derep)
Hazard & Toxicity: Exp. neoplastic agent and teratogen. LD_{50} (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: $C_9H_8O_5$
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:

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