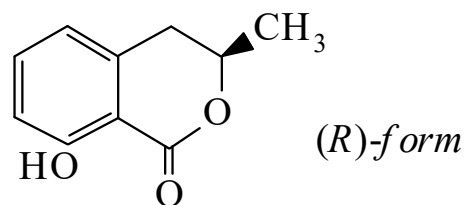




>>Entry Name: Mellein

Synonym(s): 3,4-Dihydro-8-hydroxy-3-methyl-1*H*-2-benzopyran-1-one, 9Cl. 3,4-Dihydro-8-hydroxy-3-methylisocoumarin. Ochracin



CAS Registry Number: 17397-85-2

Molecular Formula: C₁₀H₁₀O₃

Molecular Weight: 178.187

Accurate Mass: 178.062995

Percentage Composition: C 67.41%; H 5.66%; O 26.94%

Solubility: BERDY SOL: Sol. MeOH, CHCl₃, bases; fairly sol. H₂O; poorly sol. hexane

UV: [base] λ_{max} (solvent not reported) (Derep) [neutral] λ_{max} 212 (ε 20000); 246 (ε 6500); 314 (ε 4100) (MeOH) (Derep) [neutral] λ_{max} 246 (ε 6480); 315 (ε 3990) (MeOH) (Berdy) [neutral] λ_{max} 212 (ε 20000); 246 (ε 6500); 314 (ε 4100) (EtOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, ipr) 125 mg/kg ; BERDY HAZD : LD₅₀ (mus, ipr) 250 - 500 mg/kg

>>Variant: (*R*)-form

CAS Registry Number: 480-33-1

Molecular Formula: C₁₀H₁₀O₃

Molecular Weight: 178.187

Accurate Mass: 178.062995

Percentage Composition: C 67.41%; H 5.66%; O 26.94%

Biological Source: Isol. from *Aspergillus* spp. and other fungi

Physical Description: Cryst. (hexane/Et₂O)

Melting Point: Mp 51.5-52°

Optical Rotation: [α]_D -108.15 (CHCl₃)

>>Derivative: Ac

Physical Description: Cryst.

Melting Point: Mp 126-127°

>>Derivative: Me ether

Synonym(s): *O*-Methylmellein

CAS Registry Number: 16281-42-8

Biological Source: Constit. of *Septoria nodorum*

Physical Description: Cryst.

Melting Point: Mp 88-89°

Optical Rotation: [α]_D¹⁵ -250

>>Variant: (*S*)-form

CAS Registry Number: 62623-84-1

Molecular Formula: C₁₀H₁₀O₃

Molecular Weight: 178.187

Accurate Mass: 178.062995

Percentage Composition: C 67.41%; H 5.66%; O 26.94%

Biological Source: Metab. of an unidentified fungus

Melting Point: Mp 51.5-52°

Optical Rotation: [α]_D²⁵ +102 (c, 1.07 in CHCl₃)

>>Variant: (±)-form