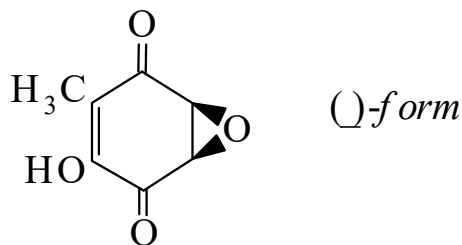




>>Entry Name: Terreic acid

Synonym(s): 3-Hydroxy-4-methyl-7-oxabicyclo[4.1.0]hept-3-ene-2,5-dione. 5,6-Epoxy-2-hydroxy-3-methyl-2-cyclohexene-1,4-dione



Molecular Formula: C₇H₆O₄

Molecular Weight: 154.122

Accurate Mass: 154.02661

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

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

UV: [acid] λ_{max} (no shifts reported) (Derep) [base] λ_{max} 253 (ε 6700); 314 (ε 4100); 383 (ε 6380) (MeOH/KOH) (Derep) [neutral] λ_{max} 213 (ε 10200); 315 (ε 6230) (MeOH) (Derep) [neutral] λ_{max} 214 (ε 10240); 316 (ε 6160) (MeOH) (Berdy) [neutral] λ_{max} 206 (E1%/1cm 42); 252 (E1%/1cm 26); 311 (E1%/1cm 39); 378 (E1%/1cm 19) (H₂O) (Berdy) [acid] λ_{max} 212 (E1%/1cm 73); 308 (E1%/1cm 50) (HCl) (Berdy) [acid] λ_{max} 215 (); 315 (ε 6600) (MeOH-HCl) (Berdy) [base] λ_{max} 254 (ε 6310); 311 (ε 4680); 386 (ε 5890) (MeOH-NAOH) (Berdy) [base] λ_{max} 218 (E1%/1cm 26); 286 (E1%/1cm 52); 312 (E1%/1cm 65) (NAOH) (Berdy)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ivn) 71 - 119 mg/kg , LD₅₀ (mus, ipr) 75 mg/kg

>>Variant: (-)-form

CAS Registry Number: 121-40-4

Molecular Formula: C₇H₆O₄

Molecular Weight: 154.122

Accurate Mass: 154.02661

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

Biological Source: Occurs in *Aspergillus terreus*

Use/Importance: Antifungal, antibacterial agent

Melting Point: Mp 124.5-125°

Optical Rotation: [α]_D²⁵ -24.9 (c, 1.8 in CHCl₃)

>>Derivative: Me ether

Melting Point: Mp 41.8-42.8°

Boiling Point: Bp₁ 80°

>>Variant: (+)-form

Molecular Formula: C₇H₆O₄

Molecular Weight: 154.122

Accurate Mass: 154.02661

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

Melting Point: Mp 124.5-125°

Optical Rotation: [α]_D²⁵ +26.5 (c, 0.5 in CHCl₃)

>>Variant: (±)-form

CAS Registry Number: 15255-24-0

Molecular Formula: C₇H₆O₄

Molecular Weight: 154.122

Accurate Mass: 154.02661

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

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 131.5-132°

References: