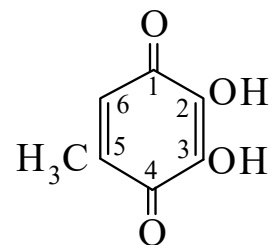




>>Entry Name: **2,3-Dihydroxy-5-methyl-1,4-benzoquinone**

Synonym(s): 2,3-Dihydroxy-5-methyl-2,5-cyclohexadiene-1,4-dione, 9Cl. 5,6-Dihydroxy-*p*-toluquinone. 3,4-Dihydroxy-2,5-toluquinone



CAS Registry Number: 825-33-2

Molecular Formula: C₇H₆O₄

Molecular Weight: 154.122

Accurate Mass: 154.02661

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

Biological Source: Prod. by *Aspergillus fumigatus* and *Penicillium spinulosum*

Physical Description: Amorph. violet substance

Melting Point: Mp 157-159°

Other Data: λ_{max} 279, 385 nm (CHCl₃)

>>Derivative: 2-Me ether

Synonym(s): 3-Hydroxy-2-methoxy-5-methyl-1,4-benzoquinone. **Fumigatin**

CAS Registry Number: 484-89-9

Molecular Formula: C₈H₈O₄

Molecular Weight: 168.149

Accurate Mass: 168.04226

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Biological Source: Prod. by *Aspergillus fumigatus*

Use/Importance: Inhibits gram-positive and -negative bacteria

Physical Description: Maroon cryst. (petrol)

Melting Point: Mp 114°

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

UV: [neutral] λ_{max} 265 (ε 13800); 450 (ε 912) (EtOH) (Berdy)

Other Data: Subl. undec.

>>Derivative: 2-Me ether, 3-Ac

Molecular Formula: C₁₀H₁₀O₅

Molecular Weight: 210.186

Accurate Mass: 210.052825

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Physical Description: Canary-yellow cryst. (petrol)

Melting Point: Mp 96-97°

>>Derivative: 2-Me ether, 5,6-epoxide

Synonym(s): 3-Hydroxy-4-methoxy-1-methyl-7-oxabicyclo[4.1.0]hept-3-ene-2,5-dione, 8Cl. **Fumigatin epoxide**. Fumigatin oxide

CAS Registry Number: 1716-19-4

Molecular Formula: C₈H₈O₅

Molecular Weight: 184.148

Accurate Mass: 184.037175

Percentage Composition: C 52.18%; H 4.38%; O 43.44%

Biological Source: From *Aphistreptus fumigatus*

Physical Description: Unstable cryst.

Melting Point: Mp 74°

Optical Rotation: [α]_D¹⁴ +28.5 (EtOH)

Solubility: BERDY SOL: Sol. MeOH, C₆H₆; poorly sol. H₂O

UV: [neutral] λ_{max} 216 (ε 11200); 330 (ε 6160) (EtOH) (Berdy) [acid] λ_{max} 315 (); 374 () (pH 1 buffer) (Berdy)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ivn) 114 - 226 mg/kg