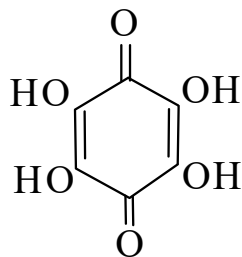




>>Entry Name: Tetrahydroxy-1,4-benzoquinone

Synonym(s): 2,3,5,6-Tetrahydroxy-2,5-cyclohexadiene-1,4-dione, 9CI. **Tetroquinone**, INN, USAN. Kelox. Terasin. HPEK 1. NSC 112931. THQ



CAS Registry Number: 319-89-1

Related CAS Registry Numbers(s): 1887-02-1 5676-48-2 123334-16-7

Molecular Formula: C₆H₄O₆

Molecular Weight: 172.094

Accurate Mass: 172.00079

Percentage Composition: C 41.88%; H 2.34%; O 55.78%

Use/Importance: Systemic keratolytic and antimicrobial agent; also shows antitrypanosomal, antiviral and carcinostatic activity. Used as indicator for titrimetric detn. of Ba, SO₄²⁽⁻⁾

Physical Description: Black plates (2M HCl)

Melting Point: Mp 300°

pKa Value: pK_{a1} 4.55; pK_{a2} 6.65 (25°)

Calculated Log P Data: Log P -2.03 (calc)

Rare Chemicals Library: S61393-2

Sigma: T6385

>>Derivative: 2,5-Di-Ac

CAS Registry Number: 20129-59-3

Molecular Formula: C₁₀H₈O₈

Molecular Weight: 256.168

Accurate Mass: 256.02192

Percentage Composition: C 46.89%; H 3.15%; O 49.97%

Physical Description: Yellow cryst. (AcOH)

Melting Point: Mp 247-248°

>>Derivative: Tetra-Ac

CAS Registry Number: 20129-61-7

Molecular Formula: C₁₄H₁₂O₁₀

Molecular Weight: 340.243

Accurate Mass: 340.04305

Percentage Composition: C 49.42%; H 3.55%; O 47.02%

Physical Description: Pale-yellow needles (MeOH)

Melting Point: Mp 172-173°

>>Derivative: 2,5-Di-Me ether

Synonym(s): 2,5-Dihydroxy-3,6-dimethoxy-1,4-benzoquinone

CAS Registry Number: 62267-71-4

Molecular Formula: C₈H₈O₆

Molecular Weight: 200.148

Accurate Mass: 200.03209

Percentage Composition: C 48.01%; H 4.03%; O 47.96%

Physical Description: Red-brown cryst. (MeOH)

Melting Point: Mp 237-238°