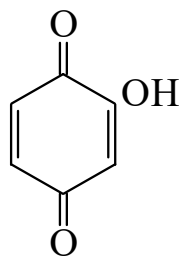




>>Entry Name: Hydroxy-1,4-benzoquinone

Synonym(s): 2-Hydroxy-2,5-cyclohexadiene-1,4-dione, 9Cl. Hydroxyquinone



CAS Registry Number: 2474-72-8

Molecular Formula: C₆H₄O₃

Molecular Weight: 124.096

Accurate Mass: 124.016045

Percentage Composition: C 58.07%; H 3.25%; O 38.68%

Physical Description: Yellow plates (petrol)

Melting Point: Mp 130-140°. Mp 124 dec.°

Other Data: Darkens on exp. to air. Negligible tautomerism to 4-Hydroxy-1,2-benzoquinone

>>Derivative: Me ether

Synonym(s): 2-Methoxy-1,4-benzoquinone

CAS Registry Number: 2880-58-2

Molecular Formula: C₇H₆O₃

Molecular Weight: 138.123

Accurate Mass: 138.031695

Percentage Composition: C 60.87%; H 4.38%; O 34.75%

Biological Source: Isol. from fruits of *Diospyros kaki*

Physical Description: Yellow needles (H₂O)

Melting Point: Mp 145°

UV: [neutral] λ_{max} 248 (ε 10470); 343 (ε 1100) (hexane) (Berdy)

Aldrich: 42485-4

>>Derivative: Me ether, 4-oxime

CAS Registry Number: 17576-99-7

Molecular Formula: C₇H₇NO₃

Molecular Weight: 153.137

Accurate Mass: 153.042594

Percentage Composition: C 54.90%; H 4.61%; N 9.15%; O 31.34%

Melting Point: Mp 176-177°

Hazard & Toxicity: LD₅₀ (mus, ipr) 120 mg/kg

>>Derivative: Et ether

Synonym(s): Ethoxy-1,4-benzoquinone

CAS Registry Number: 51767-58-9

Molecular Formula: C₈H₈O₃

Molecular Weight: 152.149

Accurate Mass: 152.047345

Percentage Composition: C 63.15%; H 5.30%; O 31.55%

Physical Description: Yellow needles

Melting Point: Mp 119-120°

References:

Jacobson, P. *et al.*, *Annalen*, 1909, **369**, 1, (*deriv*)

Willstätter, R. *et al.*, *Ber.*, 1911, **44**, 2171, (*synth*)

Gomberg, M. *et al.*, *J.A.C.S.*, 1916, **38**, 1577, (*deriv*)

Fieser, L.F., *J.A.C.S.*, 1928, **50**, 439, (*tautom*)

Flaig, W. *et al.*, *Annalen*, 1959, **626**, 215, (*ir*)

Deorhra, D.S. *et al.*, *J. Indian Chem. Soc.*, 1965, **42**, 315, (*synth, deriv*)

Blatchly, J.M. *et al.*, *J.C.S.(C)*, 1969, 1353, (*pmr*)

Hayashi, H. *et al.*, *Agric. Biol. Chem.*, 1979, **43**, 113, (*isol, deriv*)

Pratt, D.V. *et al.*, *J.O.C.*, 1987, **52**, 5053, (*deriv, synth, pmr, ir, ms*)

Keegstra, E.M.D. *et al.*, *Chem. Comm.*, 1994, 1633, (*cryst struct, deriv*)