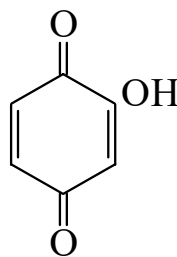




**>>Entry Name: Hydroxy-1,4-benzoquinone**

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



**CAS Registry Number:** 2474-72-8

**Molecular Formula:** C<sub>6</sub>H<sub>4</sub>O<sub>3</sub>

**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:** C<sub>7</sub>H<sub>6</sub>O<sub>3</sub>

**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 (H<sub>2</sub>O)

**Melting Point:** Mp 145°

**UV:** [neutral] λ<sub>max</sub> 248 (ε 10470); 343 (ε 1100) (hexane) (Berdy)

**Aldrich:** 42485-4

**>>Derivative:** Me ether, 4-oxime

**CAS Registry Number:** 17576-99-7

**Molecular Formula:** C<sub>7</sub>H<sub>7</sub>NO<sub>3</sub>

**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:** LD<sub>50</sub> (mus, ipr) 120 mg/kg

**>>Derivative:** Et ether

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

**CAS Registry Number:** 51767-58-9

**Molecular Formula:** C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>

**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*)  
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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*)