



>>Entry Name: **2,6-Dimethyl-1,4-benzoquinone**

Synonym(s): 2,6-Dimethyl-2,5-cyclohexadiene-1,4-dione, 9Cl. *m*-Xylo-*p*-quinone

CAS Registry Number: 527-61-7

Structure by analogy with 2,3-Dimethyl-1,4-benzoquinone, [DZW31-N](#)

Molecular Formula: C₈H₈O₂

Molecular Weight: 136.15

Accurate Mass: 136.05243

Percentage Composition: C 70.58%; H 5.92%; O 23.50%

Physical Description: Yellow needles

Melting Point: Mp 72-73°

Other Data: Sublimes

Aldrich: D14970-5

>>Derivative: 1-Oxime

CAS Registry Number: 13432-71-8

Molecular Formula: C₈H₉NO₂

Molecular Weight: 151.165

Accurate Mass: 151.063329

Percentage Composition: C 63.57%; H 6.00%; N 9.27%; O 21.17%

Physical Description: Yellow prisms (EtOH aq.)

Melting Point: Mp 175°

>>Derivative: 4-Oxime

CAS Registry Number: 4965-29-1

Molecular Formula: C₈H₉NO₂

Molecular Weight: 151.165

Accurate Mass: 151.063329

Percentage Composition: C 63.57%; H 6.00%; N 9.27%; O 21.17%

Physical Description: Yellow prisms (C₆H₆)

Melting Point: Mp 170-171°

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 452D, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 713C, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 543A, (*ir*)
Nölting, E. *et al.*, *Ber.*, 1885, **18**, 2668, (*synth*)
Flaig, W. *et al.*, *Annalen*, 1958, **618**, 117, (*uv*)
Bryce-Smith, D. *et al.*, *J.C.S.*, 1964, 873, (*synth*)
Norris, R.K. *et al.*, *Aust. J. Chem.*, 1966, **19**, 617, (*pmr*)
Rieker, A. *et al.*, *Z. Naturforsch., B*, 1969, **24**, 547, (*ir*)
Berger, S. *et al.*, *Tetrahedron*, 1972, **28**, 3123, (*cmr*)
Carpino, L.A. *et al.*, *J.O.C.*, 1989, **54**, 3303, (*synth*, *pmr*)
Omura, K., *Synthesis*, 1998, 1145-1148, (*synth*)