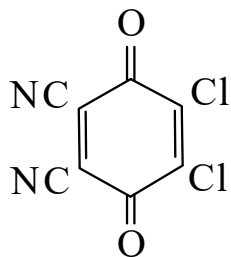




>>Entry Name: **2,3-Dichloro-5,6-dicyano-1,4-benzoquinone**

Synonym(s): 4,5-Dichloro-3,6-dioxo-1,4-cyclohexadiene-1,2-dicarbonitrile, 9Cl. DDQ



CAS Registry Number: 84-58-2

Molecular Formula: $C_8Cl_2N_2O_2$

Molecular Weight: 227.006

Accurate Mass: 225.933682

Percentage Composition: C 42.33%; Cl 31.24%; N 12.34%; O 14.10%

Use/Importance: High-potential quinone used as dehydrogenating agent. Reagent for the spectrophotometric anal. of alkaloids, and other amines. Oxidises allylmethyl and benzylmethyl ethers to carbonyl compds. Reagent for generation of radical cations for esr spectroscopy. Lewis acid catalyst for formn. of C-O and C-N bonds

Physical Description: Amber needles ($CHCl_3$)

Melting Point: Mp 215-217°

Other Data: Dec. by H_2O . The hydroquinone produced as a byprod. of oxidns. using DDQ can be readily reoxidised and reused

Hazard & Toxicity: LD₅₀ (mus, ipr) 31 mg/kg

Aldrich: D6040-0

Fluka: 35680

Sigma: D4387

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **1**, 863A, (ir)
Mitchell, P.W.D., *Can. J. Chem.*, 1963, **41**, 550, (synth, ir, uv)
Matsunaga, Y., *J. Chem. Phys.*, 1964, **41**, 1609, (ir)
Berger, S. *et al.*, *Tetrahedron*, 1972, **28**, 3123, (cmr)
Brinker, U.H. *et al.*, *Synthesis*, 1975, **10**, 671, (synth)
Lane, C.F., *Synth. Reagents*, (Pizey, J.S., Ed.), Ellis Horwood, 1977, **3**, 1, (rev)
Ohki, A. *et al.*, *Tetrahedron*, 1979, **35**, 1737, (use)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 153; **13**, 104; **16**, 120; **15**, 125; **14**, 126; **10**, 135; **9**, 148; **11**, 166; **12**, 174; **13**, 336, (use)
Lott, R.S. *et al.*, *J.O.C.*, 1980, **45**, 1151, (use)
Becker, H.D. *et al.*, *J.O.C.*, 1980, **45**, 1596, (use)
Lee, H. *et al.*, *J.O.C.*, 1983, **48**, 749, (use)
Bartos, J. *et al.*, *Pure Appl. Chem.*, 1984, **56**, 467, (use)
Newman, M.S. *et al.*, *Org. Prep. Proced. Int.*, 1985, **17**, 422, (reuse)
Abdel-Homid, M.E. *et al.*, *Talanta*, 1985, **32**, 1002, (use)
Davies, A.G. *et al.*, *Aust. J. Chem.*, 1995, **48**, 167, (use, esr)
Van den Eynde, J.J. *et al.*, *Tetrahedron*, 1995, **51**, 5813, (use, bond formn)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DEX400