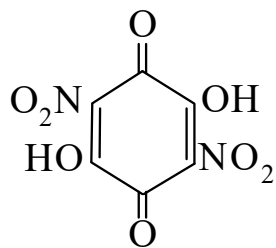




>>Entry Name: 2,5-Dihydroxy-3,6-dinitro-1,4-benzoquinone

Synonym(s): 2,5-Dihydroxy-3,6-dinitro-2,5-cyclohexadiene-1,4-dione, 9Cl. Nitranilic acid



CAS Registry Number: 479-22-1

Molecular Formula:  $C_6H_2N_2O_8$

Molecular Weight: 230.09

Accurate Mass: 229.981118

Percentage Composition: C 31.32%; H 0.88%; N 12.17%; O 55.63%

Physical Description: Golden-yellow plates (MeCN)

Melting Point: Mp 100 dec.°

pKa Value:  $pK_{a1} -3$ ;  $pK_{a2} -0.5$  (25°)

Other Data: Forms a hexahydrate, Mp 86-7°

**Hazard & Toxicity:** Explodes on heating. Forms HCN on heating

#### References:

Towns, B.W., *Biochem. J.*, 1936, **30**, 1833, (*synth*)

v. Schwerzenbach, G. *et al.*, *Helv. Chim. Acta*, 1941, **24**, 617

Parihar, D.B. *et al.*, *J. Chromatogr.*, 1966, **24**, 230, (*tlc*)

Barney, J.E. *et al.*, *Anal. Chim. Acta*, 1972, **58**, 131, (*uv, synth*)

Krogh-Andersen, E. *et al.*, *Acta Cryst. B*, 1975, **31**, 379, (*cryst struct*)

Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th edn., Van Nostrand Reinhold, 1979, 853