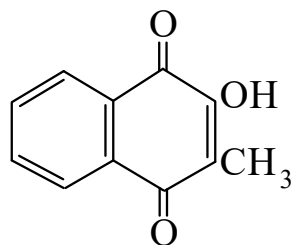




>>Entry Name: 2-Hydroxy-3-methyl-1,4-naphthoquinone

Synonym(s): 2-Hydroxy-3-methyl-1,4-naphthalenedione, 9Cl. Phthiocol



CAS Registry Number: 483-55-6

Molecular Formula: C₁₁H₈O₃

Molecular Weight: 188.182

Accurate Mass: 188.047345

Percentage Composition: C 70.21%; H 4.28%; O 25.51%

Biological Source: Pigment of human tubercle bacillus. Also isol. from *Streptococcus faecalis* and *Asplenium laciniatum*

Physical Description: Yellow needles (hexane)

Melting Point: Mp 173-174°

Solubility: BERDY SOL: Sol. MeOH, Et₂O; poorly sol. hexane, H₂O

Rare Chemicals Library: S97084-0

>>Derivative: Ac

CAS Registry Number: 6091-04-9

Molecular Formula: C₁₃H₁₀O₄

Molecular Weight: 230.22

Accurate Mass: 230.05791

Percentage Composition: C 67.82%; H 4.38%; O 27.80%

Physical Description: Pale-yellow needles (MeOH)

Melting Point: Mp 106°

>>Derivative: Thiosemicarbazone

Physical Description: Reddish-orange needles (EtOH aq.), prisms (MeOH)

Melting Point: Mp 179-180°

>>Derivative: Monoxime

CAS Registry Number: 35796-36-2

Extra CAS Registry Numbers(s): 80690-05-7

Molecular Formula: C₁₁H₉NO₃

Molecular Weight: 203.197

Accurate Mass: 203.058244

Percentage Composition: C 65.02%; H 4.46%; N 6.89%; O 23.62%

Use/Importance: Used as a 0.01M soln. in EtOH for photometric detn. of Ni (λ_{max} 510 nm, ϵ 22000)

Physical Description: Cryst. (EtOH)

Melting Point: Mp 200-201°

Solubility: Sol. EtOH

References:

- Andersen, R.J. *et al.*, *J. Biol. Chem.*, 1933, **103**, 197-201; 1939, **130**, 429-430, (*isol, synth*)
Fieser, L., *J. Biol. Chem.*, 1940, **133**, 391-396, (*synth*)
Lichstein, H.C. *et al.*, *J. Bacteriol.*, 1946, **52**, 145-146, (*props*)
Weygand, F. *et al.*, *Chem. Ber.*, 1957, **90**, 1879-1895, (*synth*)
Gaultier, N. *et al.*, *Acta Cryst.*, 1965, **19**, 919-926, (*cryst struct*)
Baum, R.H. *et al.*, *J. Biol. Chem.*, 1965, **240**, 3425-3433, (*isol*)
Gupta, R.B. *et al.*, *Curr. Sci.*, 1976, **45**, 44-46, (*isol*)
Kamini, M. *et al.*, *Analisis*, 1982, **10**, 390-392, (*synth, detn, Ni*)
Bansal, V. *et al.*, *Synth. Commun.*, 1995, **25**, 1669-1675, (*synth, pmr, ir*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, HMI000