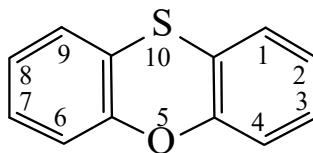




>>Entry Name: Phenoxathiin, 9Cl

Synonym(s): Phenothioxine. 9-Oxa-10-thiaanthracene. Dibenzothioxin



CAS Registry Number: 262-20-4

Molecular Formula: C₁₂H₈OS

Molecular Weight: 200.261

Accurate Mass: 200.029585

Percentage Composition: C 71.97%; H 4.03%; O 7.99%; S 16.01%

Use/Importance: Reagent for Pd

Physical Description: Plates (MeOH)

Melting Point: Mp 59°

Boiling Point: Bp₂₃ 185-187°

Other Data: H₂SO₄ → intense viol. col.

Hazard & Toxicity: Highly irritant. LD₅₀ (mus, ipr) 200 mg/kg

Aldrich: 21882-0

Rare Chemicals Library: S61479-3

>>Derivative: S-Oxide

Molecular Formula: C₁₂H₈O₂S

Molecular Weight: 216.26

Accurate Mass: 216.0245

Percentage Composition: C 66.65%; H 3.73%; O 14.80%; S 14.83%

Melting Point: Mp 152-153°

>>Derivative: S,S-Dioxide

Molecular Formula: C₁₂H₈O₃S

Molecular Weight: 232.259

Accurate Mass: 232.019415

Percentage Composition: C 62.06%; H 3.47%; O 20.67%; S 13.81%

Melting Point: Mp 146-147°

References:

Ferrario, E., *Bull. Soc. Chim. Fr.*, 1911, **9**, 536

Org. Synth., Coll. Vol., 2, 1943, 485

Gilman, H. *et al.*, *J.A.C.S.*, 1952, **74**, 2021

Breslow, D.S. *et al.*, *Multi-sulfur and Sulfur and Oxygen Five- and Six-membered Heterocycles*, (Weissberger, A., Ed.), Wiley-Interscience, Vol. 2, 1966, 864, (rev)

Isbrandt, L.R. *et al.*, *J. Magn. Reson.*, 1973, **12**, 143, (cmr)

Sharpless, M.E. *et al.*, *Org. Magn. Reson.*, 1974, **6**, 115, (pmr)

Fitzgerald, L.J. *et al.*, *Acta Cryst. C*, 1991, **47**, 381, (cryst struct)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, PDQ750