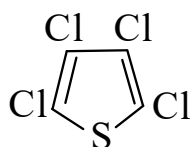




>>Entry Name: Tetrachlorothiophene

Synonym(s): Penphene



CAS Registry Number: 6012-97-1

Molecular Formula: C₄Cl₄S

Molecular Weight: 221.921

Accurate Mass: 219.847478

Percentage Composition: C 21.65%; Cl 63.90%; S 14.45%

Use/Importance: Fungicide used on tobacco crops, apparently no longer in widespread use. Nematocide. Now superseded

Melting Point: Mp 29°

Boiling Point: Bp 240-245°. Bp₂ 75-77°

Hazard & Toxicity: LD₅₀ (rat, orl) 70 mg/kg; LD₅₀ (rbt, skn) 256 mg/kg

Aldrich: 13187-3

Rare Chemicals Library: S43086-2

>>Derivative: S,S-Dioxide

CAS Registry Number: 72448-17-0

Molecular Formula: C₄Cl₄O₂S

Molecular Weight: 253.92

Accurate Mass: 251.837308

Percentage Composition: C 18.92%; Cl 55.85%; O 12.60%; S 12.63%

Use/Importance: Reactive Diels-Alder diene

Physical Description: Cryst. (hexane or by subl.)

Melting Point: Mp 91-92°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 594D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1470C, (*ir*)

Conde, S., *Synthesis*, 1976, **6**, 412, (*synth*)

Raasch, M.S., *J.O.C.*, 1980, **45**, 856, (*dioxide*)

Gupta, Y.N. *et al.*, *Tet. Lett.*, 1985, **26**, 2607, (*dioxide, use*)

Pesticide Manual, 9th edn., 1991, No. 11400

Douglas, G. *et al.*, *Acta Cryst. C*, 1993, **49**, 1197, (*cryst struct, dioxide*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, TBV750