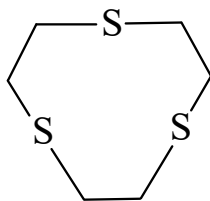




>>Entry Name: **1,4,7-Trithionane**, 9Cl, 8Cl

Synonym(s): 1,4,7-Trithiacyclononane. Triethylene trisulfide. Trithia-9-crown-3



CAS Registry Number: 6573-11-1

Molecular Formula: $C_6H_{12}S_3$

Molecular Weight: 180.359

Accurate Mass: 180.01011

Percentage Composition: C 39.96%; H 6.71%; S 53.34%

Use/Importance: Tridentate ligand for Ni, Co and Cu

Physical Description: Cryst. (MeOH or hexane)

Melting Point: Mp 84° (81-82°)

Other Data: A synthesis giving Mp 113° was erroneously reported in 1920

Aldrich: 30080-2

Fluka: 93423

Sigma: T5281

References:

- Aldrich Library of ^{13}C and 1H FT NMR Spectra*, 1992, **1**, 436B, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 357D; 422B, (*ir*)
Gerber, D. *et al.*, *J.O.C.*, 1977, **42**, 2644, (*synth, ir*)
Glass, R.S. *et al.*, *J.A.C.S.*, 1980, **102**, 5068, (*cryst struct*)
Setzer, W.N. *et al.*, *Inorg. Chem.*, 1983, **22**, 266, (*synth, ir, pmr, ms*)
Sellmann, D. *et al.*, *Angew. Chem., Int. Ed.*, 1984, **23**, 807, (*synth*)
Blower, P.J. *et al.*, *Inorg. Chem.*, 1987, **26**, 2009, (*synth, ir, pmr*)
Blom, R. *et al.*, *J.C.S. Perkin 2*, 1991, 773, (*struct*)
Lockhart, J.C. *et al.*, *J.C.S. Perkin 2*, 1992, 533, (*nmr, conformn*)