



CAS Registry Number: 18438-38-5

Molecular Formula: C₆H₇NS

Molecular Weight: 125.194

Accurate Mass: 125.029919

Percentage Composition: C 57.56%; H 5.64%; N 11.19%; S 25.61%

Physical Description: Liq.

Boiling Point: Bp₂₃ 100-104°

>>**Derivative:** S-Me; methiodide

Physical Description: Pale yellow needles (Me₂CO)

Melting Point: Mp 155-157°

>>**Derivative:** S-Me, N-oxide

Molecular Formula: C₆H₇NOS

Molecular Weight: 141.193

Accurate Mass: 141.024834

Percentage Composition: C 51.04%; H 5.00%; N 9.92%; O 11.33%; S 22.71%

Physical Description: Needles (EtOAc/hexane)

Melting Point: Mp 81°

References:

- Aldrich Library of NMR Spectra, 2nd edn.*, 1983, **2**, 640A, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 760A, (*ir*)
Jones, R.A. *et al.*, *J.C.S.*, 1958, 3610; 1960, 2937, (*synth, struct, deriv, tautom*)
Albert, A. *et al.*, *J.C.S.*, 1959, 2384, (*synth*)
Clayton, O. *et al.*, *CA*, 1967, **67**, 82111g, (*synth, N-acetoxy*)
Izquierdo, A. *et al.*, *Inf. Quim. Anal.*, 1971, **25**, 203; 1972, **26**, 271, (*pptn, photometric detn*)
Kwiatkowski, J.S., *J. Mol. Struct.*, 1971, **10**, 245, (*struct*)
Edrissi, M. *et al.*, *Microchem. J.*, 1971, **16**, 177; 526, (*synth, N-acetoxy, detn, Cu, Pd*)
Cook, M.J. *et al.*, *J.C.S. Perkin 2*, 1972, 1295, (*struct*)
Pauls, H. *et al.*, *Chem. Ber.*, 1976, **109**, 3653, (*deriv*)
Beak, P. *et al.*, *J.A.C.S.*, 1976, **98**, 171, (*struct*)
Stefaniak, L., *Org. Magn. Reson.*, 1978, **11**, 385; 1979, **12**, 379, (*nmr*)
Beak, P. *et al.*, *J.O.C.*, 1980, **45**, 1347; 1354, (*struct*)
Ohms, U. *et al.*, *Acta Cryst. B*, 1982, **38**, 831, (*cryst struct*)
Cook, I.B., *Aust. J. Chem.*, 1989, **42**, 1493, (*cmr*)
Schmidt, B. *et al.*, *J. Prakt. Chem.*, 1999, **341**, 114-120, (*use*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1993, TFP 300; HOC000