



CAS Registry Number: 1979-98-2

Molecular Formula: C₅H₆N₂O₂S

Molecular Weight: 158.181

Accurate Mass: 158.014998

Percentage Composition: C 37.97%; H 3.82%; N 17.71%; O 20.23%; S 20.27%

Melting Point: Mp 300°

Aldrich: D11480-4

>>**Derivative:** *O,O,S*-Tri-Me, *S,S*-dioxide

Synonym(s): 4,6-Dimethoxy-2-(methylsulfonyl)pyrimidine

CAS Registry Number: 113583-35-0

Molecular Formula: C₇H₁₀N₂O₄S

Molecular Weight: 218.233

Accurate Mass: 218.036128

Percentage Composition: C 38.53%; H 4.62%; N 12.84%; O 29.33%; S 14.69%

Use/Importance: Agrochemical fungicide; used in synth. of herbicides

Physical Description: Cryst. (EtOH)

Melting Point: Mp 116-119°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 835D; **2**, 821D; 822A, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1317A, (*nmr*)

Michael, A., *J. Prakt. Chem.*, 1894, **49**, 38, (*synth*)

Harwood, H.J., *CA*, 1933, **27**, 1676, (*synth*)

Dass, I.N.D. *et al.*, *Proc. - Indian Acad. Sci., Sect. A*, 1938, **8**, 145, (*deriv, synth*)

Japan. Pat., 1977, 77 07 054; *CA*, **87**, 128882c, (*use*)

Gupta, S.P. *et al.*, *Indian J. Chem., Sect. B*, 1979, **18**, 463, (*deriv, synth*)

Morelli, B., *Analyst (London)*, 1982, **107**, 282; 1983, **108**, 386; 870; 1506; 1984, **109**, 47, (*detn, Bi, Cu, Pd, Ru*)

Ohsawa, K., *Anal. Sci.*, 1985, **1**, 473, (*deriv, synth*)

Nakashima, K. *et al.*, *Chem. Pharm. Bull.*, 1985, **33**, 5380, (*deriv, use*)

Das, P.K. *et al.*, *Indian J. Chem., Sect. B*, 1985, **24**, 437, (*deriv, synth*)

Katritzky, A.R. *et al.*, *Can. J. Chem.*, 1986, **64**, 2087, (*synth, cmr*)

Gotthardt, H. *et al.*, *Chem. Ber.*, 1986, **119**, 2094, (*synth*)

Ishizumi, K. *et al.*, *Chem. Pharm. Bull.*, 1991, **39**, 2288-2300, (*tri-Me S,S-dioxide*)

Nezu, Y. *et al.*, *Pestic. Sci.*, 1996, **47**, 115-124, (*tri-Me S,S-dioxide*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, MCK500