



>>Entry Name: Methyl isothiocyanate, BSI, ISO, JMAF

ENTRY UNDER REVIEW

Synonym(s): Isothiocyanatomethane, 9CI. Methyl mustard oil. Trapex. MITC. MIT

CAS Registry Number: 556-61-6

Related CAS Registry Numbers(s): 8066-01-1 49582-15-2

MeNCS

Molecular Formula: C₂H₃NS

Molecular Weight: 73.118

Accurate Mass: 72.998619

Percentage Composition: C 32.85%; H 4.14%; N 19.16%; S 43.85%

Use/Importance: Reagent used in amino acid sequence anal.

Biological Use/Importance: Fungicide and nematocide used as a soil fumigant

Physical Description: Cryst.

Melting Point: Mp 36°

Boiling Point: Bp 119°

Other Data: *n*_D 1.5258

Hazard & Toxicity: Flammable, fl. p. 29°. Eye, skin and mucous membrane irritant. LD₅₀ (rat, orl) 97 mg/kg

Aldrich: 11277-1

Fluka: 67719

Sigma: M8632

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 873D, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1410A, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 826C, (*ir*)

Delépine, M., *Bull. Soc. Chim. Fr.*, 1908, **3**, 642, (*synth*)

Kjaer, A. *et al.*, *Acta Chem. Scand.*, 1955, **9**, 857; 1963, **17**, 2143, (*isol, ms*)

Org. Synth., Coll. Vol., **3**, 1955, 599, (*synth*)

Mathias, A. *et al.*, *Tetrahedron*, 1965, **21**, 1073, (*pmr*)

Attril, J.E. *et al.*, *Anal. Lett.*, 1970, **3**, 59, (*use*)

Waterfield, M. *et al.*, *Biochemistry*, 1970, **9**, 832, (*use*)

Anderson, D.W.W. *et al.*, *J. Mol. Struct.*, 1972, **14**, 385, (*struct*)

Fairwell, T. *et al.*, *Anal. Biochem.*, 1973, **53**, 115, (*use*)

Molina, P. *et al.*, *Synthesis*, 1982, 596, (*synth*)

Durig, J.R. *et al.*, *J. Mol. Struct.*, 1983, **100**, 241, (*ir, Raman*)

Giffard, M. *et al.*, *J.C.S. Perkin 2*, 1985, 157, (*pmr, cmr, N-15 nmr*)

Giesselmann, G. *et al.*, *Chem.-Ztg.*, 1990, **114**, 215, (*rev, synth, use, props*)

Pesticide Manual, 9th edn., 1991, No. 8390

Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A274

Verkerk, R. *et al.*, *Natural Toxicants in Food*, (ed. Watson, D.), Sheffield Academic Press/CRC, 1998, 29-53, (*rev*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, ISE000