



>>Entry Name: Ethyl isothiocyanate, 8Cl

Synonym(s): Isothiocyanatoethane, 9Cl. Ethyl mustard oil

CAS Registry Number: 542-85-8

EtNCS

Molecular Formula: C₃H₅NS

Molecular Weight: 87.145

Accurate Mass: 87.014269

Percentage Composition: C 41.35%; H 5.78%; N 16.07%; S 36.80%

Biological Source: Present as Ethyl glucosinolate [LBB69-B](#) in the seeds of *Lepidium menziesii* and *Tropaeolum peregrinum*

Physical Description: Colourless to yellowish, pungent-smelling liq.

Melting Point: Mp -5.9°

Boiling Point: Bp 131-132°

Solubility: Insol. H₂O

Density: d¹⁸ 1.003

Hazard & Toxicity: Eye, skin and respiratory tract irritant. Emits highly toxic fumes on heating to dec. or on contact with acids

Aldrich: E3390-4

Fluka: 4240

References:

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Kjaer, A. *et al.*, *Acta Chem. Scand.*, 1954, **8**, 699; 1957, **11**, 1298; 1963, **17**, 2143, (*isol, ms*)

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Maciel, G.E. *et al.*, *J. Chem. Phys.*, 1965, **69**, 3920, (*cmr*)

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Jensen, K.A. *et al.*, *Acta Chem. Scand.*, 1966, **20**, 2107, (*ms*)

Sakai, S. *et al.*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 2981, (*synth*)

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Yavari, I. *et al.*, *Org. Magn. Reson.*, 1979, **12**, 340, (*N-15 nmr*)

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