



>>Entry Name: Ethyl isocyanate

Synonym(s): Isocyanatoethane, 9CI

CAS Registry Number: 109-90-0

EtNCO

Molecular Formula: C₃H₅NO

Molecular Weight: 71.079

Accurate Mass: 71.037114

Percentage Composition: C 50.69%; H 7.09%; N 19.71%; O 22.51%

Use/Importance: Reagent for protection of Cysteine [HJQ86-N](#)

Physical Description: Pungent-smelling liq.

Boiling Point: Bp 60°

Hazard & Toxicity: LD₅₀ (mus, ivn) 56 mg/kg

Aldrich: E3330-0

Fluka: 4200

Sigma: E9629

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1401B, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 820D, (*ir*)

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 521A, (*ir*)

Gattermann, L., *Annalen*, 1888, **244**, 36, (*synth*)

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

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 383

Becker, W.D. *et al.*, *Z. Naturforsch., B*, 1970, **25**, 101, (*N-14 nmr*)

Kalinowski, H.O. *et al.*, *Angew. Chem.*, 1974, **86**, 43, (*cmr*)

U.S. Pat., 1978, 4 123 450; *CA*, **90**, 86737, (*synth*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, ELS500