



>>Entry Name: 1-Isocyanatobutane, 9CI

Synonym(s): Butyl isocyanate

CAS Registry Number: 111-36-4

$\text{H}_3\text{C}(\text{CH}_2)_3\text{NCO}$

Molecular Formula: $\text{C}_5\text{H}_9\text{NO}$

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

Boiling Point: Bp 115-120°

Hazard & Toxicity: Eye, skin and respiratory tract irritant. LD₅₀ (rat, orl) 600 mg/kg. LC₅₀ (rat, ihl) 3000 mg m⁻³. Highly flammable, fl. p. 11°

Aldrich: B9573-6

Sigma: B8259

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1402B, (nmr)

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Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 821C, (ir)

Ulrich, H. *et al.*, *Angew. Chem., Int. Ed.*, 1966, **5**, 704, (synth, props)

Martin, D. *et al.*, *Angew. Chem., Int. Ed.*, 1967, **6**, 168, (synth)

Saegusa, T. *et al.*, *Chem. Comm.*, 1977, 468, (formn)

Mitchell, W.R. *et al.*, *Chem. Ind. (London)*, 1980, 665

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Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworths, 1990, 1812