



>>Entry Name: 1-Chloro-2-isocyanatoethane, 9CI

Synonym(s): 2-Chloroethyl isocyanate, 8CI

CAS Registry Number: 1943-83-5

ClCH₂CH₂NCO

Molecular Formula: C₃H₄ClNO

Molecular Weight: 105.523

Accurate Mass: 104.998141

Percentage Composition: C 34.15%; H 3.82%; Cl 33.60%; N 13.27%; O 15.16%

Physical Description: Cryst.

Melting Point: Fp 56°

Boiling Point: Bp 135°. Bp₁₆ 42°

Density: d₂₀ 1.237

Refractive Index: n_D²⁰ 1.4493

Hazard & Toxicity: Corrosive, lachrymator

Aldrich: 24164-4

Fluka: 23040

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1406C, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 871D, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 823D, (ir)

Sadtler Standard Infrared Spectra, 23442; 42442, (ir)

Sadtler Standard NMR Spectra, 13504, (pmr)

Wenker, H., *J.A.C.S.*, 1936, **58**, 2608, (synth)

Johnson, C.K., *J.O.C.*, 1967, **32**, 1508, (synth)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, IKH000