



>>Entry Name: Chloromethyl thiocyanate, 9Cl, 8Cl

Synonym(s): Chlorothiocyاناتomethane

CAS Registry Number: 3268-79-9

ClCH₂SCN

Molecular Formula: C₂H₂ClNS

Molecular Weight: 107.563

Accurate Mass: 106.959646

Percentage Composition: C 22.33%; H 1.87%; Cl 32.96%; N 13.02%; S 29.81%

Use/Importance: Bactericide

Physical Description: Liq.

Boiling Point: Bp 185°. Bp₁₄ 63-68°

Density: d₄²⁰ 1.37

Hazard & Toxicity: Lachrymator

Aldrich: 10511-2

Fluka: 25290

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1409B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 875D, (*ir*)

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

Ger. Pat., 1963, 1 157 603; *CA*, **60**, 6787f, (*synth*)

Crowder, G.A., *J. Chem. Phys.*, 1967, **47**, 3080, (*ir*)

Crowder, G.A., *Spectrosc. Lett.*, 1986, **19**, 713, (*Raman*)