



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

Synonym(s): 2-Chloroethyl isothiocyanate. β -Chloroethyl mustard oil

CAS Registry Number: 6099-88-3

ClCH2CH2NCS

Molecular Formula: C_3H_4ClNS

Molecular Weight: 121.59

Accurate Mass: 120.975296

Percentage Composition: C 29.63%; H 3.32%; Cl 29.16%; N 11.52%; S 26.37%

Use/Importance: Reagent for synth. of *S*-contg. heterocycles

Physical Description: Unpleasant-smelling liq.

Boiling Point: $Bp_{0.13}$ 80°

Density: d_{20} 1.265

Hazard & Toxicity: Mucous membrane irritant

Aldrich: 41059-4

References:

Brintzinger, H. *et al.*, *Chem. Ber.*, 1949, **82**, 389

Outcalt, R.J., *J. Het. Chem.*, 1987, **24**, 1425, (*use, bibl*)