



>>Entry Name: 1-Chloro-3-isothiocyanatobenzene

Synonym(s): 3-Chlorophenyl isothiocyanate

CAS Registry Number: 2392-68-9

Molecular Formula: C₇H₄ClNS

Molecular Weight: 169.634

Accurate Mass: 168.975296

Percentage Composition: C 49.56%; H 2.38%; Cl 20.90%; N 8.26%; S 18.90%

Boiling Point: Bp 249-250°. Bp₂₀ 136-139°

Aldrich: 25376-6

Rare Chemicals Library: S39375-4

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 467D, (*ir*)

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **2**, 1554C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1424C, (*ir*)

Ottenbrite, R.M., *J.C.S. Perkin 1*, 1972, 88, (*synth*)

Li, Z. *et al.*, *Org. Prep. Proced. Int.*, 2000, **32**, 571-573, (*synth*)