



>>Entry Name: 1-Chloro-4-isothiocyanatobenzene, 9CI

Synonym(s): *p*-Chlorophenyl isothiocyanate. 4-Chlorophenyl isothiocyanate

CAS Registry Number: 2131-55-7

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%

Melting Point: Mp 47-48° (43-44°)

Aldrich: 25378-2

Fluka: 26001

Rare Chemicals Library: S64552-4

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1558C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 468C, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1425B, (*ir*)

Connolly, J.M. *et al.*, *J.C.S.*, 1935, 679, (*synth*)

Van der Kerk, G.J.M. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1955, **74**, 1262, (*synth*)

Cymerman-Craig, J. *et al.*, *Aust. J. Chem.*, 1960, **13**, 341, (*synth*)

Hodgkins, J.E. *et al.*, *J.O.C.*, 1964, **29**, 3098, (*synth*)

Martin, D. *et al.*, *Chem. Ber.*, 1965, **98**, 2425, (*synth*)

Fujita, H. *et al.*, *Chem. Lett.*, 1973, 883, (*synth*)

Shibanuma, T. *et al.*, *Chem. Lett.*, 1977, 573, (*synth*)

Jones, R.G. *et al.*, *Org. Magn. Reson.*, 1982, **19**, 196, (*cmr*)

Molina, P. *et al.*, *Synthesis*, 1982, 596, (*synth*)

Pak, C.S. *et al.*, *Synthesis*, 1982, 969, (*synth*)

Okajima, N. *et al.*, *J. Het. Chem.*, 1991, **28**, 177, (*synth*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, ISH000