



>>Entry Name: 1-Chloro-4-isocyanatobenzene, 9Cl

Synonym(s): *p*-Chlorophenyl isocyanate

CAS Registry Number: 104-12-1

Structure by analogy with 1-Chloro-2-isocyanatobenzene, [DXB36-D](#)

Molecular Formula: C₇H₄ClNO

Molecular Weight: 153.567

Accurate Mass: 152.998141

Percentage Composition: C 54.75%; H 2.63%; Cl 23.09%; N 9.12%; O 10.42%

Physical Description: Cryst.

Melting Point: Mp 30-31°

Boiling Point: Bp₄₅ 115-117°. Bp_{9,5} 80.6-80.9°

Hazard & Toxicity: Irritant and lachrymator. Has exploded during distillation (isolation by dist. *in vacuo* from Curtius rearrangement of corresp. azide)

Aldrich: 15227-7

Fluka: 26000

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 474B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1430C, (*ir*)

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Siefken, W., *Annalen*, 1960, **562**, 75, (*synth*)

David, D.J., *Anal. Chem.*, 1963, **35**, 37, (*ir*)

Ulrich, H. *et al.*, *J.O.C.*, 1969, **34**, 3200, (*synth*)

Ger. Pat., 1973, 2 121 183; *CA*, **78**, 29417n, (*synth*)

Yavari, I. *et al.*, *Org. Magn. Reson.*, 1979, **12**, 340, (*N-15 nmr*)

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