



>>Entry Name: 1-Fluoro-4-isocyanatobenzene, 9CI

Synonym(s): 4-Fluorophenyl isocyanate

CAS Registry Number: 1195-45-5

Structure by analogy with 1-Fluoro-2-isocyanatobenzene, [FQH12-W](#)

Molecular Formula: C₇H₄FNO

Molecular Weight: 137.113

Accurate Mass: 137.027692

Percentage Composition: C 61.32%; H 2.94%; F 13.86%; N 10.22%; O 11.67%

Physical Description: Liq.

Boiling Point: Bp₁₅ 68°

Density: d₄²⁰ 1.201

Refractive Index: n_D²⁰ 1.5216

Hazard & Toxicity: Corrosive, lachrymator. Fl. p. 41°

Aldrich: F1433-5

Fluka: 47370

Sigma: F5376

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1567B, (*nmr*)

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Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1432A, (*ir*)

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Maciel, G.E. *et al.*, *J. Chem. Phys.*, 1965, **42**, 2427, (*cmr*)

Malichenko, B.F. *et al.*, *Zh. Obshch. Khim.*, 1967, **37**, 1796; *J. Gen. Chem. USSR (Engl. Transl.)*, 1967, **37**, 1711, (*synth*)

Katritzky, A.R. *et al.*, *J.A.C.S.*, 1970, **92**, 6855, (*ir*)

Weigert, F.J. *et al.*, *J.O.C.*, 1976, **41**, 4006, (*F-19 nmr*)