



>>Entry Name: 1-Fluoro-3-isocyanatobenzene, 9CI

Synonym(s): 3-Fluorophenyl isocyanate

CAS Registry Number: 404-71-7

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

Molecular Formula: C<sub>7</sub>H<sub>4</sub>FNO

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%

Use/Importance: Herbicide intermediate

Physical Description: Liq.

Boiling Point: Bp<sub>19</sub> 69°

Density: d<sub>4</sub><sup>20</sup> 1.201

Refractive Index: n<sub>D</sub><sup>20</sup> 1.5115

Other Data: Moisture-sensitive

**Hazard & Toxicity:** Lachrymator. Fl. p. 41°

Aldrich: 15936-0

#### References:

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 1564C, (*nmr*)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 473B, (*ir*)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 1429D, (*ir*)

*Sigma-Aldrich Library of Chemical Safety Data*, 971A, (*haz*)

*U.S. Pat.*, 1954, 2 689 861; *CA*, **49**, 11712, (*synth*)

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*)