



>>Entry Name: 1-Fluoro-3-(trifluoromethyl)benzene

Synonym(s): *m*-Fluorobenzotrifluoride. $\alpha,\alpha,\alpha,3$ -Tetrafluorotoluene

CAS Registry Number: 401-80-9

Structure by analogy with 1-Fluoro-2-(trifluoromethyl)benzene, [MFZ03-G](#)

Molecular Formula: C₇H₄F₄

Molecular Weight: 164.102

Accurate Mass: 164.024912

Percentage Composition: C 51.23%; H 2.46%; F 46.31%

Physical Description: Yellow liq.

Boiling Point: Bp 101°

Refractive Index: n_D²⁰ 1.4000

Hazard & Toxicity: Highly flammable, fl. p. 7°. Irritating to eyes, respiratory system and skin

Aldrich: 21937-1

Sigma: F9875

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 145C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 997A, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 915B, (*ir*)

Suzuki, H. *et al.*, *Bull. Chem. Soc. Jpn.*, 1990, **63**, 2010, (*synth*)