



>>Entry Name: 1-Fluoro-4-(trifluoromethyl)benzene

Synonym(s): *p*-Fluorobenzotrifluoride. $\alpha,\alpha,\alpha,4$ -Tetrafluorotoluene

CAS Registry Number: 402-44-8

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: Liq.

Melting Point: Mp -42°

Boiling Point: Bp 102-105°

Refractive Index: n_D^{20} 1.4010

Hazard & Toxicity: Highly flammable, fl. p. 10°. Irritant to eyes, respiratory system and skin

Aldrich: 19535-9

Sigma: F0126

>>Derivative: Cr(0) complex

CAS Registry Number: 57821-01-9

Physical Description: Dark green solid

Melting Point: Mp 60.5-61°

Boiling Point: Subl._{0.001} 56°

Other Data: Air-stable for several days

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **2**, 148B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 998A, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 917A, (*ir*)

Graves, V. *et al.*, *Inorg. Chem.*, 1976, **15**, 577, (*complex*)

Kobayashi, Y. *et al.*, *J. Fluorine Chem.*, 1986, **32**, 467, (*synth*)

Naumann, D. *et al.*, *J. Fluorine Chem.*, 1990, **47**, 283, (*synth, F-19 nmr*)