



>>Entry Name: 2-Fluoro-6-(trifluoromethyl)benzoic acid

Synonym(s): $\alpha,\alpha,\alpha,6$ -Tetrafluoro-*o*-toluic acid, 8Cl

CAS Registry Number: 32890-94-1

Structure by analogy with 2-Fluoro-3-(trifluoromethyl)benzoic acid, [KNS71-Y](#)

Molecular Formula: C₈H₄F₄O₂

Molecular Weight: 208.112

Accurate Mass: 208.014742

Percentage Composition: C 46.17%; H 1.94%; F 36.52%; O 15.38%

Melting Point: Mp 83-84°

Aldrich: 33080-9

>>Derivative: Chloride

CAS Registry Number: 109227-12-5

Molecular Formula: C₈H₃ClF₄O

Molecular Weight: 226.557

Accurate Mass: 225.980854

Percentage Composition: C 42.41%; H 1.33%; Cl 15.65%; F 33.54%; O 7.06%

Physical Description: No phys. props. reported

Other Data: Not well documented but comly. available

>>Derivative: Nitrile

Synonym(s): 2-Cyano-1-fluoro-3-(trifluoromethyl)benzene

CAS Registry Number: 133116-83-3

Molecular Formula: C₈H₃F₄N

Molecular Weight: 189.112

Accurate Mass: 189.020161

Percentage Composition: C 50.81%; H 1.60%; F 40.18%; N 7.41%

Other Data: Comly. available; no synth. reported in the lit.

Other: Oakwood 2047

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **2**, 1092B, (*nmr*)

Schlosser, M. *et al.*, *Synlett*, 1990, 747, (*synth*, *pmr*)