



**>>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:** C<sub>8</sub>H<sub>4</sub>F<sub>4</sub>O<sub>2</sub>

**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:** C<sub>8</sub>H<sub>3</sub>ClF<sub>4</sub>O

**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:** C<sub>8</sub>H<sub>3</sub>F<sub>4</sub>N

**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 <sup>13</sup>C and <sup>1</sup>H FT NMR Spectra*, 1992, **2**, 1092B, (*nmr*)

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