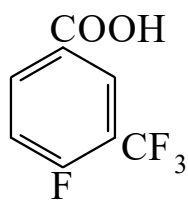




>>Entry Name: 4-Fluoro-3-(trifluoromethyl)benzoic acid, 9Cl, 8Cl



**CAS Registry Number:** 67515-55-3

**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 115-116°

**Aldrich:** 45526-1

>>Derivative: Fluoride

**CAS Registry Number:** 67515-54-2

**Molecular Formula:** C<sub>8</sub>H<sub>3</sub>F<sub>5</sub>O

**Molecular Weight:** 210.103

**Accurate Mass:** 210.010405

**Percentage Composition:** C 45.73%; H 1.44%; F 45.21%; O 7.62%

**Boiling Point:** Bp<sub>18</sub> 57-60°

>>Derivative: Chloride

**CAS Registry Number:** 67515-56-4

**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%

**Boiling Point:** Bp<sub>6</sub> 80-90°

>>Derivative: Amide

**CAS Registry Number:** 67515-57-5

**Molecular Formula:** C<sub>8</sub>H<sub>5</sub>F<sub>4</sub>NO

**Molecular Weight:** 207.127

**Accurate Mass:** 207.030726

**Percentage Composition:** C 46.39%; H 2.43%; F 36.69%; N 6.76%; O 7.72%

**Physical Description:** Cryst.

**Melting Point:** Mp 87-88°

>>Derivative: Nitrile

**CAS Registry Number:** 67515-59-7

**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%

**Physical Description:** Cryst.

**Melting Point:** Mp 67-68°

**Other Data:** Sublimes

#### References:

*Ger. Pat.*, 1978, 2 757 406; *CA*, **89**, 109081r, (*synth, amide, nitrile*)

Yonezawa, N. *et al.*, *Synth. Commun.*, 1996, **26**, 1575, (*nitrile*)