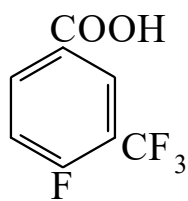




>>Entry Name: 4-Fluoro-3-(trifluoromethyl)benzoic acid, 9Cl, 8Cl



CAS Registry Number: 67515-55-3

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 115-116°

Aldrich: 45526-1

>>Derivative: Fluoride

CAS Registry Number: 67515-54-2

Molecular Formula: C₈H₃F₅O

Molecular Weight: 210.103

Accurate Mass: 210.010405

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

Boiling Point: Bp₁₈ 57-60°

>>Derivative: Chloride

CAS Registry Number: 67515-56-4

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%

Boiling Point: Bp₆ 80-90°

>>Derivative: Amide

CAS Registry Number: 67515-57-5

Molecular Formula: C₈H₅F₄NO

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: C₈H₃F₄N

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*)