



>>Entry Name: 3-Fluorobenzoic acid

CAS Registry Number: 455-38-9

Structure by analogy with 2-Fluorobenzoic acid, [DTM63-K](#)

Molecular Formula: C₇H₅FO₂

Molecular Weight: 140.114

Accurate Mass: 140.027358

Percentage Composition: C 60.01%; H 3.60%; F 13.56%; O 22.84%

Physical Description: Leaflets (H₂O)

Melting Point: Mp 124°

pKa Value: pK_a 3.85 (25°)

Aldrich: F660-5

Fluka: 46590

Sigma: F9877

>>Derivative: Me ester

CAS Registry Number: 455-68-5

Molecular Formula: C₈H₇FO₂

Molecular Weight: 154.14

Accurate Mass: 154.043008

Percentage Composition: C 62.34%; H 4.58%; F 12.33%; O 20.76%

Melting Point: Mp -10°

Boiling Point: Bp 197°

>>Derivative: Et ester

CAS Registry Number: 451-02-5

Molecular Formula: C₉H₉FO₂

Molecular Weight: 168.167

Accurate Mass: 168.058658

Percentage Composition: C 64.28%; H 5.39%; F 11.30%; O 19.03%

Boiling Point: Bp 209°

Aldrich: 28351-7

Sigma: F5761

>>Derivative: Isopropyl ester

CAS Registry Number: 2711-76-4

Molecular Formula: C₁₀H₁₁FO₂

Molecular Weight: 182.194

Accurate Mass: 182.074308

Percentage Composition: C 65.92%; H 6.09%; F 10.43%; O 17.56%

Boiling Point: Bp₁₈ 100-101°

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 831-34-5

Molecular Formula: C₁₁H₁₃FO₂

Molecular Weight: 196.221

Accurate Mass: 196.089958

Percentage Composition: C 67.33%; H 6.68%; F 9.68%; O 16.31%

Boiling Point: Bp_{0.3} 50-51°

>>Derivative: Fluoride

Molecular Formula: C₇H₄F₂O

Molecular Weight: 142.105

Accurate Mass: 142.023021

Percentage Composition: C 59.17%; H 2.84%; F 26.74%; O 11.26%

Boiling Point: Bp₃₀ 56-60°