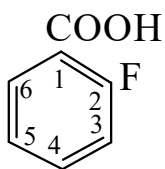




>>Entry Name: 2-Fluorobenzoic acid



CAS Registry Number: 445-29-4

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: Needles (H₂O)

Melting Point: Mp 126.5°

Density: d₄²⁵ 1.46

pKa Value: pK_a 3.47 (25°)

Aldrich: 41224-4

Fluka: 46580

Sigma: F9375

>>Derivative: Me ester

CAS Registry Number: 394-35-4

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 -20°

Boiling Point: Bp 209°. Bp₁₄ 89-90°

Rare Chemicals Library: S43645-3

>>Derivative: Et ester

CAS Registry Number: 443-26-5

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%

Melting Point: Mp 221°

>>Derivative: Isopropyl ester

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 113°

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 69038-73-9

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_{0.4} 78-79°