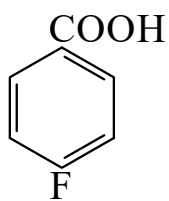




>>Entry Name: 4-Fluorobenzoic acid



CAS Registry Number: 456-22-4

Molecular Formula:  $C_7H_5FO_2$

Molecular Weight: 140.114

Accurate Mass: 140.027358

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

Use/Importance: Used in etching. Reference material used in elemental microanalysis

Physical Description: Prisms ( $H_2O$ )

Melting Point: Mp  $185^\circ$

pKa Value:  $pK_a$  4.15 ( $25^\circ$ )

Aldrich: 12838-4

Fluka: 46600

Sigma: F7003

>>Derivative: Me ester

CAS Registry Number: 403-33-8

Molecular Formula:  $C_8H_7FO_2$

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  $4.5^\circ$

Boiling Point: Bp  $198^\circ$

Aldrich: 12070-7

>>Derivative: Et ester

CAS Registry Number: 451-46-7

Molecular Formula:  $C_9H_9FO_2$

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  $26^\circ$

Boiling Point: Bp  $211^\circ$

Refractive Index:  $n_D^{25.7}$  1.4707

Aldrich: 10264-4

Fluka: 46610

>>Derivative: Isopropyl ester

CAS Registry Number: 2928-09-8

Molecular Formula:  $C_{10}H_{11}FO_2$

Molecular Weight: 182.194

Accurate Mass: 182.074308

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

Boiling Point: Bp<sub>22</sub>  $96^\circ$

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 58656-98-7

Molecular Formula:  $C_{11}H_{13}FO_2$

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<sub>0.4</sub>  $51-52^\circ$