



>>Entry Name: 2,6-Difluorobenzoic acid

CAS Registry Number: 385-00-2

Molecular Formula: $C_7H_4F_2O_2$

Molecular Weight: 158.104

Accurate Mass: 158.017936

Percentage Composition: C 53.18%; H 2.55%; F 24.03%; O 20.24%

Physical Description: Cryst. (CCl₄)

Melting Point: Mp 161-162°

pKa Value: pK_a 2.27 (25°, H₂O)

Aldrich: 19003-9

Fluka: 36884

Sigma: D2027

>>Derivative: Me ester

CAS Registry Number: 13671-00-6

Molecular Formula: $C_8H_6F_2O_2$

Molecular Weight: 172.131

Accurate Mass: 172.033586

Percentage Composition: C 55.82%; H 3.51%; F 22.07%; O 18.59%

Physical Description: Liq.

Boiling Point: Bp₁₅ 90-91°

>>Derivative: Et ester

CAS Registry Number: 19064-14-3

Molecular Formula: $C_9H_8F_2O_2$

Molecular Weight: 186.158

Accurate Mass: 186.049236

Percentage Composition: C 58.07%; H 4.33%; F 20.41%; O 17.19%

Physical Description: Oil

>>Derivative: Chloride

CAS Registry Number: 18063-02-0

Molecular Formula: $C_7H_3ClF_2O$

Molecular Weight: 176.55

Accurate Mass: 175.984048

Percentage Composition: C 47.62%; H 1.71%; Cl 20.08%; F 21.52%; O 9.06%

Physical Description: Liq.

Boiling Point: Bp₁₅ 76-79°

Aldrich: 24940-8

Fluka: 36916

>>Derivative: Amide

CAS Registry Number: 18063-03-1

Molecular Formula: $C_7H_5F_2NO$

Molecular Weight: 157.119

Accurate Mass: 157.03392

Percentage Composition: C 53.51%; H 3.21%; F 24.18%; N 8.91%; O 10.18%

Physical Description: Needles (C₆H₆)

Melting Point: Mp 144.5-145.5°

Aldrich: 28227-8

Fluka: 36901

Sigma: D1157