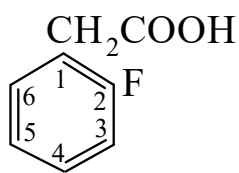




>>>Entry Name: 2-Fluorophenylacetic acid

Synonym(s): 2-Fluorobenzeneacetic acid, 9Cl. *o*-Fluorophenylacetic acid, 8Cl. 2-Fluorophenylethanoic acid. *o*-Fluoro- α -toluic acid



CAS Registry Number: 451-82-1

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%

Physical Description: Cryst. (CHCl₃)

Melting Point: Mp 59°

pK_a Value: pK_a 4.09 (20°, H₂O)

Aldrich: 20894-9

Fluka: 47340

>>Derivative: Et ester

CAS Registry Number: 584-74-7

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: Bp₂₄ 135-136°. Bp_{0.5} 65°

>>Derivative: Chloride

Molecular Formula: C₈H₆ClFO

Molecular Weight: 172.586

Accurate Mass: 172.00912

Percentage Composition: C 55.68%; H 3.50%; Cl 20.54%; F 11.01%; O 9.27%

Boiling Point: Bp 203-204°

>>Derivative: Amide

CAS Registry Number: 326-63-6

Molecular Formula: C₈H₈FNO

Molecular Weight: 153.156

Accurate Mass: 153.058992

Percentage Composition: C 62.74%; H 5.26%; F 12.40%; N 9.15%; O 10.45%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 158-159°

>>Derivative: Nitrile

CAS Registry Number: 326-62-5

Molecular Formula: C₈H₆FN

Molecular Weight: 135.14

Accurate Mass: 135.048427

Percentage Composition: C 71.10%; H 4.47%; F 14.06%; N 10.36%

Boiling Point: Bp 230-235°. Bp₁₀ 102°

Aldrich: 19934-6

Sigma: F4626

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1002C; 1487B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 150C; 429B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1319D; 1402C, (*ir*)

Olah, G. *et al.*, *J.O.C.*, 1957, **22**, 879; *J.C.S.*, 1963, 5437, (*synth*)

Shapiro, R.H., *Org. Mass Spectrom.*, 1968, **1**, 907, (*ms*)