>>**Entry Name: 3-Fluorophenylacetic acid**
Synonym(s): 3-Fluorobenzeneacetic acid, 9CI. *m*-Fluorophenylacetic acid, 8CI. 3-Fluorophenylethanoic acid. *m*-Fluoro-α-toluic acid

CAS Registry Number: 331-25-9
Structure by analogy with 2-Fluorophenylacetic acid, FGJ09-S

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%
Physical Description: Cryst. (petrol)
Melting Point: Mp 48°
pKa Value: pK_a 4.13 (25°, H_2O)

Aldrich: 24804-5
Fluka: 47345

>>**Derivative:** Et ester

CAS Registry Number: 587-47-3
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_{28} 126-129°. Bp_{12} 110-111°

>>**Derivative:** Amide

CAS Registry Number: 370-45-6
Molecular Formula: C_8H_8FNO
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%
Melting Point: Mp 141°

>>**Derivative:** Nitrile

CAS Registry Number: 501-00-8
Molecular Formula: C_8H_6FN
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 229-230°. Bp_{10} 124-126°
Other Data: Bp also given as 109°/12 mm
Aldrich: F1335-5

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1007B; 1490A, *(nmr)*
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 431D, *(ir)*
Sadtler Standard C-13 NMR Spectra, 7005, *(cmr)*
Sadtler Standard Infrared Spectra, 28158, *(ir)*
Elderfield, R.C. *et al.*, *J.A.C.S.*, 1960, **82**, 1975, *(synth)*
Taft, R.W. *et al.*, *J.A.C.S.*, 1963, **85**, 709, *(synth)*
Shapiro, R.H.*, Org. Mass Spectrom.*, 1968, **1**, 907, *(ms)*