>>**Entry Name: Pentafluorophenylacetic acid**
Synonym(s): 2,3,4,5,6-Pentafluorobenzeneacetic acid, 9Cl

CAS Registry Number: 653-21-4
$(C_6F_5)CH_2COOH$

Molecular Formula: $C_8H_3F_5O_2$
Molecular Weight: 226.102
Accurate Mass: 226.00532
Percentage Composition: C 42.50%; H 1.34%; F 42.01%; O 14.15%
Physical Description: Cryst. (petrol)
Melting Point: Mp 109°

Aldrich: 24808-8
Sigma: P6536

>>**Derivative:** Et ester

CAS Registry Number: 784-35-0
Molecular Formula: $C_{10}H_7F_5O_2$
Molecular Weight: 254.156
Accurate Mass: 254.03662
Percentage Composition: C 47.26%; H 2.78%; F 37.38%; O 12.59%
Boiling Point: Bp_{14} 94-96°

>>**Derivative:** Chloride

CAS Registry Number: 832-72-4
Molecular Formula: $C_8H_2ClF_5O$
Molecular Weight: 244.548
Accurate Mass: 243.971432
Percentage Composition: C 39.29%; H 0.82%; Cl 14.50%; F 38.84%; O 6.54%
Boiling Point: Bp_{29} 90-95°

>>**Derivative:** Amide

Molecular Formula: $C_8H_4F_5NO$
Molecular Weight: 225.118
Accurate Mass: 225.021304
Percentage Composition: C 42.68%; H 1.79%; F 42.20%; N 6.22%; O 7.11%
Physical Description: Cryst. ($EtOH/C_6H_6$)
Melting Point: Mp 187-188°

>>**Derivative:** Nitrile
Synonym(s): Pentafluorophenylacetonitrile. (Cyanomethyl)pentafluorobenzene

CAS Registry Number: 653-30-5
Molecular Formula: $C_8H_2F_5N$
Molecular Weight: 207.102
Accurate Mass: 207.010739
Percentage Composition: C 46.40%; H 0.97%; F 45.87%; N 6.76%
Melting Point: Mp 38-38.5°
Boiling Point: Bp_8 105°
Aldrich: 24809-6

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1040B; 1500C, *(nmr)*
Barbour, A.K. *et al.*, *J.C.S.*, 1961, 808, *(synth, ir)*
Org. Synth., 1977, **57**, 80, *(nitrile)*
Bordwell, F.G. *et al.*, *J.O.C.*, 1988, **53**, 780, *(nitrile)*