



>>Entry Name: Pentafluorophenylacetic acid

Synonym(s): 2,3,4,5,6-Pentafluorobenzeneacetic acid, 9CI

CAS Registry Number: 653-21-4

(C₆F₅)CH₂COOH

Molecular Formula: C₈H₃F₅O₂

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: C₁₀H₇F₅O₂

Molecular Weight: 254.156

Accurate Mass: 254.03662

Percentage Composition: C 47.26%; H 2.78%; F 37.38%; O 12.59%

Boiling Point: Bp₁₄ 94-96°

>>Derivative: Chloride

CAS Registry Number: 832-72-4

Molecular Formula: C₈H₂ClF₅O

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: Bp₂₉ 90-95°

>>Derivative: Amide

Molecular Formula: C₈H₄F₅NO

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/C₆H₆)

Melting Point: Mp 187-188°

>>Derivative: Nitrile

Synonym(s): Pentafluorophenylacetonitrile. (Cyanomethyl)pentafluorobenzene

CAS Registry Number: 653-30-5

Molecular Formula: C₈H₂F₅N

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: Bp₈ 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*)