



>>Entry Name: Difluorophenylacetic acid, 9CI

Synonym(s): α,α -Difluorobenzeneacetic acid

CAS Registry Number: 360-03-2

PhCF₂COOH

Molecular Formula: C₈H₆F₂O₂

Molecular Weight: 172.131

Accurate Mass: 172.033586

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

Physical Description: Cryst. (CFCl₃ or petrol)

Melting Point: Mp 76-77° (62-63°)

>>Derivative: Me ester

CAS Registry Number: 56071-96-6

Molecular Formula: C₉H₈F₂O₂

Molecular Weight: 186.158

Accurate Mass: 186.049236

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

Boiling Point: Bp₂₀ 100-101°

>>Derivative: Et ester

CAS Registry Number: 2248-46-6

Molecular Formula: C₁₀H₁₀F₂O₂

Molecular Weight: 200.185

Accurate Mass: 200.064886

Percentage Composition: C 60.00%; H 5.03%; F 18.98%; O 15.98%

Physical Description: Oil

Boiling Point: Bp₂₀ 100°

>>Derivative: Chloride

Molecular Formula: C₈H₅ClF₂O

Molecular Weight: 190.576

Accurate Mass: 189.999698

Percentage Composition: C 50.42%; H 2.64%; Cl 18.60%; F 19.94%; O 8.40%

Boiling Point: Bp₁₅ 67-68°

>>Derivative: Amide

CAS Registry Number: 383-19-7

Molecular Formula: C₈H₇F₂NO

Molecular Weight: 171.146

Accurate Mass: 171.04957

Percentage Composition: C 56.14%; H 4.12%; F 22.20%; N 8.18%; O 9.35%

Physical Description: Cryst. (C₆H₆ or H₂O)

Melting Point: Mp 114-115°

Rare Chemicals Library: S11799-4

>>Derivative: Nitrile

Synonym(s): α,α -Difluorobenzeneacetonitrile. Cyanodifluorophenylmethane. α -Cyano- α,α -difluorotoluene

CAS Registry Number: 2002-72-4

Molecular Formula: C₈H₅F₂N

Molecular Weight: 153.131

Accurate Mass: 153.039005

Percentage Composition: C 62.75%; H 3.29%; F 24.81%; N 9.15%

Physical Description: Liq.

Boiling Point: Bp₉₈ 94-95°

References:

Middleton, W.J. *et al.*, *J.O.C.*, 1980, **45**, 2883, (*synth*)

Taguchi, T. *et al.*, *Tet. Lett.*, 1986, **27**, 6103, (*synth, ester*)

Parisi, M.F. *et al.*, *J.O.C.*, 1995, **60**, 5174, (*Me ester, synth, pmr, F-19 nmr, ir, cmr*)

Hagele, G. *et al.*, *J. Fluorine Chem.*, 1996, **76**, 15-19, (*Et ester, nitrile*)

Sato, K. *et al.*, *Chem. Pharm. Bull.*, 1999, **47**, 1013-1016, (*Et ester, synth, ir, pmr, F-19 nmr*)