



>>Entry Name: 3,4-Difluorophenylacetic acid

Synonym(s): 3,4-Difluorobenzeneacetic acid, 9CI

CAS Registry Number: 658-93-5

Related CAS Registry Numbers(s): 658-99-1 121639-61-0 129409-55-8 210530-71-5

Molecular Formula: $C_8H_6F_2O_2$

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. (hexane)

Melting Point: Mp 46-50° (40-42°)

Aldrich: 29043-2

Fluka: 36950

Sigma: D6156

>>Derivative: Nitrile

CAS Registry Number: 658-99-1

Molecular Formula: $C_8H_5F_2N$

Molecular Weight: 153.131

Accurate Mass: 153.039005

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

Boiling Point: Bp₁₃ 110-120°

Aldrich: 26452-0

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, 1405A

Baltzly, R. *et al.*, *J.O.C.*, 1961, **26**, 2353-2355, (*synth*)

Mattiello, L. *et al.*, *J.C.S. Perkin 2*, 1990, 1041-1044, (*Et ester, pmr*)