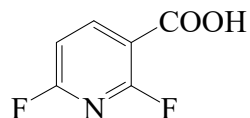




>>Entry Name: 2,6-Difluoro-3-pyridinecarboxylic acid, 9CI

Synonym(s): 2,6-Difluoronicotinic acid



CAS Registry Number: 171178-50-0

Molecular Formula: $C_6H_3F_2NO_2$

Molecular Weight: 159.092

Accurate Mass: 159.013185

Percentage Composition: C 45.30%; H 1.90%; F 23.88%; N 8.80%; O 20.11%

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 167-170°

>>Derivative: Me ester

CAS Registry Number: 117671-02-0

Molecular Formula: $C_7H_5F_2NO_2$

Molecular Weight: 173.119

Accurate Mass: 173.028835

Percentage Composition: C 48.57%; H 2.91%; F 21.95%; N 8.09%; O 18.48%

Physical Description: Oil

>>Derivative: Amide

CAS Registry Number: 171178-51-1

Molecular Formula: $C_6H_4F_2N_2O$

Molecular Weight: 158.107

Accurate Mass: 158.029169

Percentage Composition: C 45.58%; H 2.55%; F 24.03%; N 17.72%; O 10.12%

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 107-108°

References:

- Rewcastle, G.W. *et al.*, *J. Med. Chem.*, 1996, **39**, 1823-1835, (*amide, synth, pmr, cmr*)
Terauchi, H. *et al.*, *Chem. Pharm. Bull.*, 1997, **45**, 1027-1038, (*synth, ir, pmr*)
Shutske, G.M. *et al.*, *J. Het. Chem.*, 1997, **34**, 789-795, (*synth, ir, pmr*)
Hirokawa, Y. *et al.*, *Chem. Pharm. Bull.*, 2000, **48**, 1847-1853, (*Me ester*)