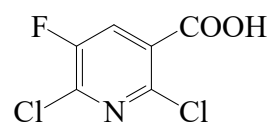




>>Entry Name: 2,6-Dichloro-5-fluoro-3-pyridinecarboxylic acid, 9Cl

Synonym(s): 2,6-Dichloro-5-fluoronicotinic acid



CAS Registry Number: 82671-06-5

Molecular Formula: $C_6H_2Cl_2FNO_2$

Molecular Weight: 209.991

Accurate Mass: 208.944661

Percentage Composition: C 34.32%; H 0.96%; Cl 33.77%; F 9.05%; N 6.67%; O 15.24%

Use/Importance: Intermed. for synth of naphthyridine antibacterial agents

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 155-156°

>>Derivative: Et ester

CAS Registry Number: 82671-03-2

Molecular Formula: $C_8H_6Cl_2FNO_2$

Molecular Weight: 238.045

Accurate Mass: 236.975961

Percentage Composition: C 40.37%; H 2.54%; Cl 29.79%; F 7.98%; N 5.88%; O 13.44%

Physical Description: Yellow liq.

Boiling Point: Bp₃ 95-97°

>>Derivative: Chloride

CAS Registry Number: 96568-02-4

Molecular Formula: C_6HCl_3FNO

Molecular Weight: 228.437

Accurate Mass: 226.910773

Percentage Composition: C 31.55%; H 0.44%; Cl 46.56%; F 8.32%; N 6.13%; O 7.00%

Use/Importance: Intermed. for synth. of naphthyridine antibacterial agents

Physical Description: Liq.

Boiling Point: Bp_{0.8} 80°

>>Derivative: Amide

CAS Registry Number: 113237-20-0

Molecular Formula: $C_6H_3Cl_2FN_2O$

Molecular Weight: 209.006

Accurate Mass: 207.960645

Percentage Composition: C 34.48%; H 1.45%; Cl 33.93%; F 9.09%; N 13.40%; O 7.65%

Physical Description: Solid (Et₂O)

Melting Point: Mp 163-164°

>>Derivative: Nitrile

Synonym(s): 2,6-Dichloro-3-cyano-5-fluoropyridine

CAS Registry Number: 82671-02-1

Molecular Formula: $C_6HCl_2FN_2$

Molecular Weight: 190.991

Accurate Mass: 189.95008

Percentage Composition: C 37.73%; H 0.53%; Cl 37.12%; F 9.95%; N 14.67%

Physical Description: Solid (Et₂O/hexane)

Melting Point: Mp 91-93° (87-88°)

References:

Ger. Pat., 1986, 3 508 816; *CA*, **105**, 191059v, (*chloride*)

Miyamoto, T. *et al.*, *Chem. Pharm. Bull.*, 1987, **35**, 2280; 1990, **38**, 3211, (*synth, amide, nitrile, pmr*)

Eur. Pat., 1989, 3 33 020; *CA*, **112**, 118659f, (*nitrile*)

U.S. Pat., 1993, 5 204 478; *CA*, **119**, 139119q, (*chloride*)