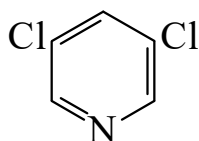




>>Entry Name: 3,5-Dichloropyridine, 9Cl



CAS Registry Number: 2457-47-8

Molecular Formula: C₅H₃Cl₂N

Molecular Weight: 147.991

Accurate Mass: 146.964253

Percentage Composition: C 40.58%; H 2.04%; Cl 47.91%; N 9.46%

Use/Importance: Bactericide and fungicide

Physical Description: Leaflets (EtOH aq.)

Melting Point: Mp 64-65°

pKa Value: pK_a 0.67 (25°)

Hazard & Toxicity: LD₅₀ (mus, ipr) 1180 mg/kg

Aldrich: D7380-4

>>Derivative: N-Oxide

CAS Registry Number: 15177-57-8

Molecular Formula: C₅H₃Cl₂NO

Molecular Weight: 163.99

Accurate Mass: 162.959168

Percentage Composition: C 36.62%; H 1.84%; Cl 43.24%; N 8.54%; O 9.76%

Physical Description: Needles (petrol)

Melting Point: Mp 109-110°

Boiling Point: Subl.₁₅ 110°

pKa Value: pK_a -0.94

>>Derivative: N-Fluoro

CAS Registry Number: 107264-06-2

Molecular Formula: C₅H₃Cl₂FN⁽⁺⁾

Molecular Weight: 166.989

Accurate Mass: 165.962656

Percentage Composition: C 35.96%; H 1.81%; Cl 42.46%; F 11.38%; N 8.39%

Use/Importance: Fluorinating agent

Physical Description: Cryst. (MeCN/Et₂O) (as triflate salt)

Melting Point: Mp 118.5-121° (sealed tube) (triflate salt)

Other Data: CAS no. refers to triflate

Aldrich: 37822-4

Fluka: 35849

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