



>>Entry Name: 3,4,5-Trichloro-2-pyridinecarboxylic acid, 9Cl

Synonym(s): 3,4,5-Trichloropicolinic acid, 8Cl

CAS Registry Number: 5439-04-3

Molecular Formula: C₆H₂Cl₃NO₂

Molecular Weight: 226.445

Accurate Mass: 224.91511

Percentage Composition: C 31.82%; H 0.89%; Cl 46.97%; N 6.19%; O 14.13%

Physical Description: Needles (H₂O)

Melting Point: Mp 164-165° (155°)

>>Derivative: Me ester

Molecular Formula: C₇H₄Cl₃NO₂

Molecular Weight: 240.472

Accurate Mass: 238.93076

Percentage Composition: C 34.96%; H 1.68%; Cl 44.23%; N 5.82%; O 13.31%

Physical Description: Plates (MeOH or H₂O)

Melting Point: Mp 84-85°

>>Derivative: Et ester

Molecular Formula: C₈H₆Cl₃NO₂

Molecular Weight: 254.499

Accurate Mass: 252.94641

Percentage Composition: C 37.76%; H 2.38%; Cl 41.79%; N 5.50%; O 12.57%

Melting Point: Mp 34-35°

>>Derivative: Ph ester

Molecular Formula: C₁₂H₆Cl₃NO₂

Molecular Weight: 302.543

Accurate Mass: 300.94641

Percentage Composition: C 47.64%; H 2.00%; Cl 35.15%; N 4.63%; O 10.58%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 93-94°

>>Derivative: Chloride

Molecular Formula: C₆HCl₄NO

Molecular Weight: 244.891

Accurate Mass: 242.881222

Percentage Composition: C 29.43%; H 0.41%; Cl 57.91%; N 5.72%; O 6.53%

Melting Point: Mp 24-25°

Boiling Point: Bp₁₂ 135-136°

References:

Sell, W.J. *et al.*, *J.C.S.*, 1905, **87**, 799-804, (*synth, Me ester*)

Graf, R. *et al.*, *J. Prakt. Chem.*, 1937, **148**, 13-23, (*synth, esters, chloride*)