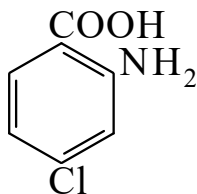




>>Entry Name: 2-Amino-4-chlorobenzoic acid, 9Cl

Synonym(s): 4-Chloroanthranilic acid, 8Cl



CAS Registry Number: 89-77-0

Molecular Formula: C₇H₆ClNO₂

Molecular Weight: 171.583

Accurate Mass: 171.008706

Percentage Composition: C 49.00%; H 3.52%; Cl 20.66%; N 8.16%; O 18.65%

Physical Description: Thick yellowish needles (EtOH aq.)

Melting Point: Mp 219-223°. Mp 239-240°

pKa Value: pK_{a1} 1.21; pK_{a2} 4.44 (25°, 0.1M KCl)

Aldrich: A4546-7

Fluka: 7353

>>Derivative: Me ester

CAS Registry Number: 5900-58-3

Molecular Formula: C₈H₈ClNO₂

Molecular Weight: 185.609

Accurate Mass: 185.024356

Percentage Composition: C 51.77%; H 4.34%; Cl 19.10%; N 7.55%; O 17.24%

Physical Description: Needles

Melting Point: Mp 68-69°

Fluka: 7378

>>Derivative: Et ester

CAS Registry Number: 60064-34-8

Molecular Formula: C₉H₁₀ClNO₂

Molecular Weight: 199.636

Accurate Mass: 199.040006

Percentage Composition: C 54.15%; H 5.05%; Cl 17.76%; N 7.02%; O 16.03%

Physical Description: Needles

Melting Point: Mp 41°

>>Derivative: Amide

CAS Registry Number: 5900-59-4

Molecular Formula: C₇H₇ClN₂O

Molecular Weight: 170.598

Accurate Mass: 170.02469

Percentage Composition: C 49.28%; H 4.14%; Cl 20.78%; N 16.42%; O 9.38%

Physical Description: Plates

Melting Point: Mp 181-182°

>>Derivative: Nitrile

Synonym(s): 5-Chloro-2-cyanoaniline

CAS Registry Number: 38487-86-4

Molecular Formula: C₇H₅ClN₂

Molecular Weight: 152.583

Accurate Mass: 152.014125

Percentage Composition: C 55.10%; H 3.30%; Cl 23.24%; N 18.36%

Physical Description: Needles (petrol/EtOAc)

Melting Point: Mp 162°