



>>Entry Name: 4-Amino-2-chlorophenol, 9Cl
ENTRY UNDER REVIEW

CAS Registry Number: 3964-52-1

Molecular Formula: C₆H₆ClNO
Molecular Weight: 143.572
Accurate Mass: 143.013791
Percentage Composition: C 50.19%; H 4.21%; Cl 24.69%; N 9.76%; O 11.14%
Physical Description: Needles (H₂O)
Melting Point: Mp 153°
pKa Value: pK_{a2} 9.16 (25°)

Aldrich: 43733-6

>>Derivative: *N*-Ac

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 144°

>>Derivative: *O,N*-Di-Ac

Molecular Formula: C₁₀H₁₀ClNO₃
Molecular Weight: 227.647
Accurate Mass: 227.034921
Percentage Composition: C 52.76%; H 4.43%; Cl 15.57%; N 6.15%; O 21.08%
Physical Description: Needles (H₂O)
Melting Point: Mp 124°

>>Derivative: Me ether

Synonym(s): 3-Chloro-4-methoxybenzenamine, 9Cl. 3-Chloro-4-methoxyaniline. 3-Chloro-*p*-anisidine. 4-Amino-2-chloroanisole

CAS Registry Number: 5345-54-0
Molecular Formula: C₇H₈ClNO
Molecular Weight: 157.599
Accurate Mass: 157.029441
Percentage Composition: C 53.35%; H 5.12%; Cl 22.50%; N 8.89%; O 10.15%
Physical Description: Needles
Melting Point: Mp 62°
Hazard & Toxicity: Eye and skin irritant. LD₅₀ (rat, orl) 550 mg/kg

Aldrich: 22860-5

>>Derivative: Me ether; hydrochloride

Melting Point: Mp 278-279°

>>Derivative: Me ether, *N*-Ac

Synonym(s): 3-Chloro-4-methoxyacetanilide. 3-Chloro-*p*-anisidide. 4-Acetamido-2-chloroanisole

CAS Registry Number: 7073-42-9
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 (H₂O)
Melting Point: Mp 94°
Rare Chemicals Library: S94152-2