



>>Entry Name: 4-Amino-2-chlorobenzoic acid, 9Cl, 8Cl

CAS Registry Number: 2457-76-3

Molecular Formula: $C_7H_6ClNO_2$

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%

Use/Importance: Exhibits herbicidal and coccicidal props.

Melting Point: Mp 213°

Hazard & Toxicity: LD₅₀ (mus, ipr) 500 mg/kg

Aldrich: 21771-9

Fluka: 7355

Sigma: A3504

>>Derivative: Hydrochloride

Melting Point: Mp 185°

>>Derivative: Me ester

CAS Registry Number: 46004-37-9

Molecular Formula: $C_8H_8ClNO_2$

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%

Melting Point: Mp 107-108°

>>Derivative: Et ester

CAS Registry Number: 16017-69-9

Molecular Formula: $C_9H_{10}ClNO_2$

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%

Melting Point: Mp 110-111°

>>Derivative: Nitrile

Synonym(s): 3-Chloro-4-cyanoaniline

CAS Registry Number: 20925-27-3

Molecular Formula: $C_7H_5ClN_2$

Molecular Weight: 152.583

Accurate Mass: 152.014125

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

Physical Description: Cryst. (C_6H_6)

Melting Point: Mp 162-163°

Aldrich: 27901-3

Fluka: 7390

>>Derivative: N-Ac

CAS Registry Number: 38667-55-9

Molecular Formula: $C_9H_8ClNO_3$

Molecular Weight: 213.62

Accurate Mass: 213.019271

Percentage Composition: C 50.60%; H 3.77%; Cl 16.60%; N 6.56%; O 22.47%

Melting Point: Mp 206°

References: