



>>Entry Name: **3-Amino-2,5-dichlorobenzoic acid**, 9Cl, 8Cl

Synonym(s): Chloramben, BSI. Amiben. Vegiben

CAS Registry Number: 133-90-4

Molecular Formula: $C_7H_5Cl_2NO_2$

Molecular Weight: 206.027

Accurate Mass: 204.969733

Percentage Composition: C 40.81%; H 2.45%; Cl 34.42%; N 6.80%; O 15.53%

Use/Importance: Preemergence herbicide

Physical Description: Purplish-white powder

Melting Point: Mp 200-201°

Other Data: Numerous *N*-acyl derivs. have also been used as herbicides

Hazard & Toxicity: LD₅₀ (rat, orl) 3500 mg/kg

Rare Chemicals Library: S45830-9

Sigma: A5509

>>Derivative: Me ester

CAS Registry Number: 7286-84-2

Molecular Formula: $C_8H_7Cl_2NO_2$

Molecular Weight: 220.054

Accurate Mass: 218.985383

Percentage Composition: C 43.67%; H 3.21%; Cl 32.22%; N 6.37%; O 14.54%

Use/Importance: Herbicide

Melting Point: Mp 58-60°. Mp 63-64°

Supelco: R47-4305

>>Derivative: Amide

Synonym(s): 3-Amino-2,5-dichlorobenzamide. Chlorambenamide

CAS Registry Number: 2280-93-5

Molecular Formula: $C_7H_6Cl_2N_2O$

Molecular Weight: 205.043

Accurate Mass: 203.985717

Percentage Composition: C 41.00%; H 2.95%; Cl 34.58%; N 13.66%; O 7.80%

Use/Importance: Herbicide

Physical Description: Cryst. (H₂O)

Melting Point: Mp 162-163°

>>Derivative: *N*-Ac

Molecular Formula: $C_9H_7Cl_2NO_3$

Molecular Weight: 248.065

Accurate Mass: 246.980298

Percentage Composition: C 43.58%; H 2.84%; Cl 28.58%; N 5.65%; O 19.35%

Use/Importance: Herbicide

Melting Point: Mp 215-217°

>>Derivative: *N,N*-Di-Me

Molecular Formula: $C_9H_9Cl_2NO_2$

Molecular Weight: 234.081

Accurate Mass: 233.001033

Percentage Composition: C 46.18%; H 3.88%; Cl 30.29%; N 5.98%; O 13.67%

Melting Point: Mp 194-197 dec.°

References:

U.S. Pat., 1958, 3 014 063; *CA*, **56**, 8643e, (*synth*)

U.S. Pat., 1973, 3 703 546; *CA*, **78**, 71690, (*synth*)

Berkheiser, V.E. *et al.*, *Weed Sci.*, 1976, **24**, 107, (*ir, uv*)

U.K. Pat., 1977, 1 453 405; *CA*, **86**, 106182, (*synth*)

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Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, AJM000