



>>Entry Name: 3,6-Dichloro-2-hydroxybenzoic acid

Synonym(s): 3,6-Dichlorosalicylic acid

CAS Registry Number: 3401-80-7

Related CAS Registry Numbers(s): 1982-69-0 2300-66-5 8065-43-8 8068-77-7 10007-85-9

Molecular Formula: $C_7H_4Cl_2O_3$

Molecular Weight: 207.012

Accurate Mass: 205.953749

Percentage Composition: C 40.61%; H 1.95%; Cl 34.25%; O 23.19%

Melting Point: Mp 187°

>>Derivative: Me ether

Synonym(s): 3,6-Dichloro-2-methoxybenzoic acid. 3,6-Dichloro-*o*-anisic acid. **Dicamba**, ANSI, BSI, ISO, WSSA

CAS Registry Number: 1918-00-9

Molecular Formula: $C_8H_6Cl_2O_3$

Molecular Weight: 221.039

Accurate Mass: 219.969399

Percentage Composition: C 43.47%; H 2.74%; Cl 32.08%; O 21.71%

Use/Importance: Herbicide

Physical Description: Solid (pentane)

Melting Point: Mp 114-116°

pKa Value: pK_a 1.95

Other Data: Also used as Na, K and dimethylammonium salts

Hazard & Toxicity: LD₅₀ (rat, orl) 1700 mg/kg

Sigma: D5417

>>Derivative: Me ether, Me ester

Synonym(s): Methyl 3,6-dichloro-2-methoxybenzoate. Disugran, ANSI. Dicamba-methyl, BSI, ISO

CAS Registry Number: 6597-78-0

Molecular Formula: $C_9H_8Cl_2O_3$

Molecular Weight: 235.066

Accurate Mass: 233.985049

Percentage Composition: C 45.99%; H 3.43%; Cl 30.16%; O 20.42%

Use/Importance: Plant growth regulator

Boiling Point: Bp_{2.4} 115°

Supelco: R47-3520

References:

Berzovskii, M. *et al.*, *CA*, 1971, **76**, 136758, (*deriv*)

Suzuki, H.K. *et al.*, *Anal. Methods Pestic. Plant Growth Regul.*, 1978, **10**, 305, (*rev, props*)

Pagani, G. *et al.*, *Farmaco, Ed. Sci.*, 1978, **33**, 189, (*synth, activity*)

Smith, G. *et al.*, *Aust. J. Chem.*, 1983, **36**, 2175, (*cryst struct*)

Durham, D.R. *et al.*, *J. Bacteriol.*, 1987, **169**, 2889, (*synth*)

Pesticide Manual, 9th edn., 1991, 245

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MEL500