



>>Entry Name: 3,5-Dichloro-4-hydroxybenzoic acid

CAS Registry Number: 3336-41-2

Molecular Formula: C₇H₄Cl₂O₃

Molecular Weight: 207.012

Accurate Mass: 205.953749

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

Biological Source: Prod. by *Bjerkandera* sp. BOS55

Physical Description: Cryst. (AcOH)

Melting Point: Mp 268-269°

pKa Value: pK_a 9.31

Hazard & Toxicity: LD₅₀ (mus, ipr) 650 mg/kg

Aldrich: D6400-7

>>Derivative: Me ester

CAS Registry Number: 3337-59-5

Molecular Formula: C₈H₆Cl₂O₃

Molecular Weight: 221.039

Accurate Mass: 219.969399

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

Physical Description: Needles

Melting Point: Mp 147°

>>Derivative: Et ester

CAS Registry Number: 17302-82-8

Molecular Formula: C₉H₈Cl₂O₃

Molecular Weight: 235.066

Accurate Mass: 233.985049

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

Physical Description: Needles (EtOH)

Melting Point: Mp 116°

>>Derivative: Me ether

Synonym(s): 3,5-Dichloro-4-methoxybenzoic acid. 3,5-Dichloroanisic acid, 8Cl

CAS Registry Number: 37908-97-7

Molecular Formula: C₈H₆Cl₂O₃

Molecular Weight: 221.039

Accurate Mass: 219.969399

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

Biological Source: Prod. by *Bjerkandera* spp. and found in a soil sample associated with *Lepista nuda*

Melting Point: Mp 202°

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **2**, 230A, (ir)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1144C, (nmr)
Datta, R.L. *et al.*, *J.A.C.S.*, 1919, **41**, 2023
Blakey, W. *et al.*, *J.C.S.*, 1927, 2865, (deriv)
Tarbell, H.S. *et al.*, *J.A.C.S.*, 1942, **64**, 1066, (synth)
Org. Synth., *Coll. Vol.*, 3, 1955, 267, (synth)
Fischer, A. *et al.*, *J.C.S.(B)*, 1967, 686
Swarts, H.J. *et al.*, *Phytochemistry*, 1996, **42**, 1699, (isol, ms)