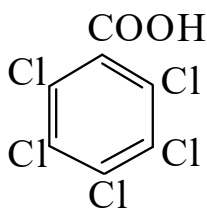




>>Entry Name: Pentachlorobenzoic acid, 9Cl, 8Cl

Synonym(s): Perchlorobenzoic acid



CAS Registry Number: 1012-84-6

Molecular Formula: $C_7HCl_5O_2$

Molecular Weight: 294.347

Accurate Mass: 291.841915

Percentage Composition: C 28.56%; H 0.34%; Cl 60.22%; O 10.87%

Physical Description: Needles (C_6H_6)

Melting Point: Mp 208°

Hazard & Toxicity: LD₅₀ (mus, ipr) 178 mg/kg

Rare Chemicals Library: S81223-4

>>Derivative: Me ester

CAS Registry Number: 51877-62-4

Molecular Formula: $C_8H_3Cl_5O_2$

Molecular Weight: 308.374

Accurate Mass: 305.857565

Percentage Composition: C 31.16%; H 0.98%; Cl 57.48%; O 10.38%

Melting Point: Mp 97°

>>Derivative: Chloride

CAS Registry Number: 1825-23-6

Molecular Formula: C_7Cl_6O

Molecular Weight: 312.793

Accurate Mass: 309.808027

Percentage Composition: C 26.88%; Cl 68.01%; O 5.12%

Physical Description: Plates (EtOH)

Melting Point: Mp 87°

Rare Chemicals Library: S82975-7

>>Derivative: Amide

CAS Registry Number: 29956-85-2

Molecular Formula: $C_7H_2Cl_5NO$

Molecular Weight: 293.362

Accurate Mass: 290.857899

Percentage Composition: C 28.66%; H 0.69%; Cl 60.42%; N 4.77%; O 5.45%

Melting Point: Mp 268°

References:

Deacon, G.B. *et al.*, *Aust. J. Chem.*, 1967, **20**, 1587, (*synth*)

Weidenbruch, M. *et al.*, *Chem. Ber.*, 1970, **103**, 510, (*synth*)