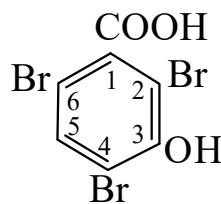




>>Entry Name: 2,4,6-Tribromo-3-hydroxybenzoic acid



CAS Registry Number: 14348-40-4

Molecular Formula: C₇H₃Br₃O₃

Molecular Weight: 374.811

Accurate Mass: 371.823228

Percentage Composition: C 22.43%; H 0.81%; Br 63.96%; O 12.81%

Physical Description: Needles + ½ H₂O (H₂O), anhyd. at 100°

Melting Point: Mp 147-148°

Aldrich: 43953-3

>>Derivative: Me ester

Molecular Formula: C₈H₅Br₃O₃

Molecular Weight: 388.838

Accurate Mass: 385.838878

Percentage Composition: C 24.71%; H 1.30%; Br 61.65%; O 12.34%

Physical Description: Plates or needles (petrol)

Melting Point: Mp 119-121°

>>Derivative: Amide

Molecular Formula: C₇H₄Br₃NO₂

Molecular Weight: 373.826

Accurate Mass: 370.839212

Percentage Composition: C 22.49%; H 1.08%; Br 64.12%; N 3.75%; O 8.56%

Melting Point: Mp 221°

>>Derivative: Nitrile

Synonym(s): 2,4,6-Tribromo-3-cyanophenol

CAS Registry Number: 54582-94-4

Molecular Formula: C₇H₂Br₃NO

Molecular Weight: 355.811

Accurate Mass: 352.828647

Percentage Composition: C 23.63%; H 0.57%; Br 67.37%; N 3.94%; O 4.50%

Physical Description: Yellow needles (petrol)

Melting Point: Mp 168°

>>Derivative: Nitrile, 3-Ac

Molecular Formula: C₉H₄Br₃NO₂

Molecular Weight: 397.848

Accurate Mass: 394.839212

Percentage Composition: C 27.17%; H 1.01%; Br 60.25%; N 3.52%; O 8.04%

Physical Description: Yellowish-white plates (EtOH aq.)

Melting Point: Mp 156-158°

>>Derivative: Ac

Molecular Formula: C₉H₅Br₃O₄

Molecular Weight: 416.848

Accurate Mass: 413.833793

Percentage Composition: C 25.93%; H 1.21%; Br 57.51%; O 15.35%

Physical Description: Cryst. (MeOH or CHCl₃/petrol)

Melting Point: Mp 192-193°

>>Derivative: 4-Methylbenzenesulfonyl

CAS Registry Number: 14753-52-7

Melting Point: Mp 189-191°