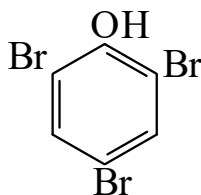




>>Entry Name: 2,4,6-Tribromophenol, 9Cl, 8Cl

ENTRY UNDER REVIEW

Synonym(s): Bromol



CAS Registry Number: 118-79-6

Related CAS Registry Numbers(s): 2666-53-7 3784-04-1 78697-30-0

Extra CAS Registry Numbers(s): 25376-38-9

Molecular Formula: C₆H₃Br₃O

Molecular Weight: 330.801

Accurate Mass: 327.833398

Percentage Composition: C 21.79%; H 0.91%; Br 72.46%; O 4.84%

Biological Source: Isol. from a marine acorn worm. Also found in the green alga *Ulva lactuca*. Isol. from molluses and crustaceans

Use/Importance: Stronger antiseptic than phenol or thymol. Used as 5-7% soln. in KOH for gravimetric detn. of Pd(II) or Pt(II) (in NH₃ soln., as [M(NH₃)₄][OC₆H₂Br₃]₂).

Flavour component of seafood, imparts an intense shrimp-like flavour

Physical Description: Needles (EtOH), prisms (C₆H₆)

Melting Point: Mp 87-89°

Boiling Point: Subl. 95-96°

Solubility: Sol. alkalis, EtOH, petrol

UV: [neutral] λ_{max} 288 (); 297 () (EtOH) (Berdy)

Hazard & Toxicity: Potent irritant. LD₅₀ (rat, orl) 2000 mg/kg

Aldrich: 13771-5

Fluka: 90730

Supelco: 44-2304

>>Derivative: Ac

CAS Registry Number: 607-95-4

Molecular Formula: C₈H₅Br₃O₂

Molecular Weight: 372.838

Accurate Mass: 369.843963

Percentage Composition: C 25.77%; H 1.35%; Br 64.29%; O 8.58%

Physical Description: Plates or needles (EtOH)

Melting Point: Mp 87°

>>Derivative: Benzoyl

CAS Registry Number: 24003-13-2

Molecular Formula: C₁₃H₇Br₃O₂

Molecular Weight: 434.909

Accurate Mass: 431.859613

Percentage Composition: C 35.90%; H 1.62%; Br 55.12%; O 7.36%

Physical Description: Needles (EtOH)

Melting Point: Mp 81°

>>Derivative: 4-Methylbenzenesulfonyl

CAS Registry Number: 2437-48-1

Physical Description: Cryst. (EtOH)

Melting Point: Mp 113°