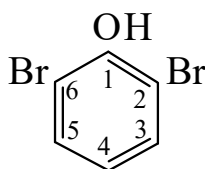




>>Entry Name: 2,6-Dibromophenol, 9Cl, 8Cl
ENTRY UNDER REVIEW



CAS Registry Number: 608-33-3

Molecular Formula: C₆H₄Br₂O

Molecular Weight: 251.905

Accurate Mass: 249.902887

Percentage Composition: C 28.61%; H 1.60%; Br 63.44%; O 6.35%

Biological Source: Constit. of the marine hemichordate *Balanoglossus biminensis*

Use/Importance: Important flavour component of marine fish, molluses and crustaceans

Physical Description: Needles (H₂O)

Melting Point: Mp 56-57°

Boiling Point: Bp₂₁ 162°

Solubility: BERDY SOL: Sol. EtOH, Et₂O

pKa Value: pK_a 6.67 (25°)

UV: [neutral] λ_{max} 279 (ε 2180); 286 (ε 2130) (EtOH) (Berdy) [base] λ_{max} 305 () (EtOH-NaOH) (Berdy)

Other Data: Sublimes

Aldrich: 25201-8

Fluka: 34269

Supelco: R42-8414

>>Derivative: Ac

CAS Registry Number: 28165-72-2

Molecular Formula: C₈H₆Br₂O₂

Molecular Weight: 293.942

Accurate Mass: 291.913452

Percentage Composition: C 32.69%; H 2.06%; Br 54.37%; O 10.89%

Melting Point: Mp 46°

>>Derivative: Benzoyl

Molecular Formula: C₁₃H₈Br₂O₂

Molecular Weight: 356.013

Accurate Mass: 353.929102

Percentage Composition: C 43.86%; H 2.26%; Br 44.89%; O 8.99%

Melting Point: Mp 68°

>>Derivative: Me ether

Synonym(s): 1,3-Dibromo-2-methoxybenzene. 2,6-Dibromoanisole

Molecular Formula: C₇H₆Br₂O

Molecular Weight: 265.932

Accurate Mass: 263.918537

Percentage Composition: C 31.62%; H 2.27%; Br 60.09%; O 6.02%

Melting Point: Mp 13°

Boiling Point: Bp₃₄ 143-145°

>>Derivative: Et ether

Synonym(s): 1,3-Dibromo-2-ethoxybenzene. 2,6-Dibromophenetole

Molecular Formula: C₈H₈Br₂O

Molecular Weight: 279.959

Accurate Mass: 277.934187

Percentage Composition: C 34.32%; H 2.88%; Br 57.08%; O 5.71%

Melting Point: Mp 40.5°

References: