



>>Entry Name: 2,4-Dibromophenol, 9Cl, 8Cl
ENTRY UNDER REVIEW

CAS Registry Number: 615-58-7

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: Isol. from the acorn worms *Balanoglossus carnosus* and *Ptychodera* sp. Commonly found in molluses and crustaceans

Melting Point: Mp 40°

Boiling Point: Bp₁₁ 154°

pKa Value: pK_a 7.79 (25°)

Hazard & Toxicity: LD₅₀ (mus, orl) 282 mg/kg

Aldrich: 25816-4

Fluka: 34270

Rare Chemicals Library: S56460-5

Supelco: R42-8410

>>Derivative: Ac

CAS Registry Number: 36914-79-1

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 36°

>>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 97.5°

>>Derivative: Me ether

Synonym(s): 2,4-Dibromo-1-methoxybenzene. 2,4-Dibromoanisole

CAS Registry Number: 21702-84-1

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%

Biological Source: Constit. of the red alga *Polysiphonia sphaerocarpa*

Melting Point: Mp 61.5°

Boiling Point: Bp 272°

Aldrich: 30118-3

>>Derivative: Et ether

Synonym(s): 2,4-Dibromo-1-ethoxybenzene. 2,4-Dibromophenetole

CAS Registry Number: 38751-57-4

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 53.5°

References: