



>>Entry Name: 4,5-Dibromo-1,2-benzenediol, 9CI

Synonym(s): 4,5-Dibromocatechol

CAS Registry Number: 2563-26-0

Molecular Formula: C₆H₄Br₂O₂

Molecular Weight: 267.904

Accurate Mass: 265.897802

Percentage Composition: C 26.90%; H 1.50%; Br 59.65%; O 11.94%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 122°

>>Derivative: Di-Ac

Molecular Formula: C₁₀H₈Br₂O₄

Molecular Weight: 351.979

Accurate Mass: 349.918932

Percentage Composition: C 34.12%; H 2.29%; Br 45.40%; O 18.18%

Melting Point: Mp 110°

>>Derivative: Dibenzyl ether

CAS Registry Number: 206995-42-8

Molecular Formula: C₂₀H₁₆Br₂O₂

Molecular Weight: 448.153

Accurate Mass: 445.991702

Percentage Composition: C 53.60%; H 3.60%; Br 35.66%; O 7.14%

Physical Description: Cryst. (CH₂Cl₂)

Melting Point: Mp 144.5-155.5°

References:

Kohn, M., *J.A.C.S.*, 1951, **73**, 480, (*synth*)

van Nostrum, C.F. *et al.*, *J.A.C.S.*, 1995, **117**, 9957-9965, (*synth, ir, pmr*)

Hu, M. *et al.*, *J. Med. Chem.*, 1998, **41**, 1789-1802, (*dibenzyl ether, synth, ir, pmr, cmr, ms*)