



>>Entry Name: 4-Amino-2,6-dibromophenol, 9CI

CAS Registry Number: 609-21-2

Molecular Formula: C₆H₅Br₂NO

Molecular Weight: 266.92

Accurate Mass: 264.913786

Percentage Composition: C 27.00%; H 1.89%; Br 59.87%; N 5.25%; O 5.99%

Physical Description: Needles (C₆H₆)

Melting Point: Mp 191-193°

Aldrich: 32392-6

>>Derivative: *N*-Ac

CAS Registry Number: 63558-07-6

Molecular Formula: C₈H₇Br₂NO₂

Molecular Weight: 308.957

Accurate Mass: 306.924351

Percentage Composition: C 31.10%; H 2.28%; Br 51.73%; N 4.53%; O 10.36%

Physical Description: Leaflets + 1H₂O

Melting Point: Mp 173-174°

>>Derivative: Me ether

Synonym(s): 3,5-Dibromo-4-methoxyaniline. 3,5-Dibromo-*p*-anisidine

CAS Registry Number: 41727-70-2

Molecular Formula: C₇H₇Br₂NO

Molecular Weight: 280.946

Accurate Mass: 278.929436

Percentage Composition: C 29.93%; H 2.51%; Br 56.88%; N 4.99%; O 5.69%

Melting Point: Mp 66°

>>Derivative: Me ether, *N*-Ac

Molecular Formula: C₉H₉Br₂NO₂

Molecular Weight: 322.984

Accurate Mass: 320.940001

Percentage Composition: C 33.47%; H 2.81%; Br 49.48%; N 4.34%; O 9.91%

Physical Description: Needles (EtOH)

Melting Point: Mp 198°

>>Derivative: Et ether

Synonym(s): 3,5-Dibromo-4-ethoxyaniline. 3,5-Dibromo-*p*-phenetidine

CAS Registry Number: 52765-17-0

Molecular Formula: C₈H₉Br₂NO

Molecular Weight: 294.973

Accurate Mass: 292.945086

Percentage Composition: C 32.58%; H 3.08%; Br 54.18%; N 4.75%; O 5.42%

Physical Description: Needles

Melting Point: Mp 107°

>>Derivative: Et ether, *N*-Ac

Molecular Formula: C₁₀H₁₁Br₂NO₂

Molecular Weight: 337.01

Accurate Mass: 334.955651

Percentage Composition: C 35.64%; H 3.29%; Br 47.42%; N 4.16%; O 9.49%

Melting Point: Mp 198°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 532B, (*nmr*)

Bargellini, G. *et al.*, *Atti Accad. Naz. Lincei, Cl. Sci. Fis., Mat. Nat., Rend.*, 1930, **11**, 574, (*synth*)

Gillois, M. *et al.*, *Bull. Soc. Chim. Fr.*, 1954, 112

Fujita, E. *et al.*, *Yakugaku Zasshi*, 1957, **77**, 750, (*synth*)