



>>Entry Name: 4-Amino-1-butanol

CAS Registry Number: 13325-10-5

H2NCH2CH2CH2CH2OH

Molecular Formula: C4H11NO

Molecular Weight: 89.137

Accurate Mass: 89.084064

Percentage Composition: C 53.90%; H 12.44%; N 15.71%; O 17.95%

Physical Description: Oil

Boiling Point: Bp 206°. Bp₃₄ 125°

Solubility: Sol. EtOH, insol. Et₂O

Other Data: Forms a hydrate in water. Absorbs CO₂ and H₂O from air

Hazard & Toxicity: LD₅₀ (rat, orl) 1150 mg/kg

Aldrich: 17833-0

Fluka: 7191

>>Derivative: Picrate

Melting Point: Mp 86.6-88.6°

>>Derivative: Me ether

Synonym(s): 4-Methoxy-1-butylamine. 1-Amino-4-methoxybutane

CAS Registry Number: 34039-36-6

Molecular Formula: C5H13NO

Molecular Weight: 103.164

Accurate Mass: 103.099714

Percentage Composition: C 58.21%; H 12.70%; N 13.58%; O 15.51%

Boiling Point: Bp 142-145°

Solubility: Sol. H₂O, EtOH, Et₂O

>>Derivative: *N,N*-Di-Me

Synonym(s): 4-(Dimethylamino)-1-butanol, 9CI

CAS Registry Number: 13330-96-6

Molecular Formula: C6H15NO

Molecular Weight: 117.191

Accurate Mass: 117.115364

Percentage Composition: C 61.49%; H 12.90%; N 11.95%; O 13.65%

Physical Description: Oil

Boiling Point: Bp 186-189°. Bp₁₄ 80-81°

>>Derivative: *N,N*-Dibutyl

CAS Registry Number: 94473-23-1

Molecular Formula: C12H27NO

Molecular Weight: 201.351

Accurate Mass: 201.209264

Percentage Composition: C 71.58%; H 13.52%; N 6.96%; O 7.95%

Boiling Point: Bp₄₀ 172-175°

References:

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Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 538A, (*nmr*)
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Henry, L., *Ber.*, 1900, **33**, 3170, (*synth*)
Lunsford, C.D. *et al.*, *J.O.C.*, 1957, **22**, 1225, (*N,N*-dibutyl)
Kaluszyner, A. *et al.*, *J.O.C.*, 1961, **26**, 3536, (*deriv*)
Hoffman, R.V. *et al.*, *J.C.S. Perkin I*, 1989, 1375, (*deriv*)
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