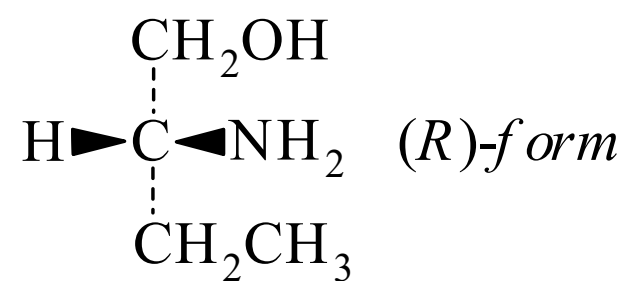




>>Entry Name: 2-Amino-1-butanol, 9CI



CAS Registry Number: 96-20-8

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%

Use/Importance: Cheaply available intermed. which can be readily resolved on an industrial scale

Other Data: The parent amine has too low a m.w. to give cryst. salts with most acids and the *O*-benzyl deriv. is recommended as a resolving agent (Touet *et al*)

Hazard & Toxicity: Fl. p. 74° (oc). LD₅₀ (mus, orl) 2300 mg/kg

Aldrich: A4380-4

Rare Chemicals Library: S44045-0

>>Variant: (*R*)-form

CAS Registry Number: 5856-63-3

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%

Aldrich: 30708-4

Fluka: 7180

Sigma: A4795

>>Derivative: Oxalate

Optical Rotation: $[\alpha]_{\text{D}}^{20} -11.3$ (H₂O)

>>Derivative: *O*-Benzyl

Molecular Formula: C₁₁H₁₇NO

Molecular Weight: 179.261

Accurate Mass: 179.131014

Percentage Composition: C 73.70%; H 9.56%; N 7.81%; O 8.93%

Use/Importance: Resolving agent

Physical Description: Viscous oil

Optical Rotation: $[\alpha]_{\text{D}} -18.9$ (c, 1.5 in EtOH)

>>Derivative: *O*-Benzyl; hydrochloride

Physical Description: Cryst.

Optical Rotation: $[\alpha]_{\text{D}} -18$ (c, 1.1 in EtOH)

>>Variant: (*S*)-form

CAS Registry Number: 5856-62-2

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%

Boiling Point: Bp₁₁ 80°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +9.8$ (H₂O)

Aldrich: 13252-7

Fluka: 7178

>>Derivative: Oxalate

Melting Point: Mp 190-192°

Optical Rotation: $[\alpha]$