



>>Entry Name: 3-Amino-1-propanol

Synonym(s): 3-Hydroxypropylamine. Propanolamine

CAS Registry Number: 156-87-6

Related CAS Registry Numbers(s): 18600-41-4 29833-41-8 29833-46-3

H2NCH2CH2CH2OH

Molecular Formula: C3H9NO

Molecular Weight: 75.11

Accurate Mass: 75.068414

Percentage Composition: C 47.97%; H 12.08%; N 18.65%; O 21.30%

Melting Point: Mp 11°

Boiling Point: Bp 188°. Bp_{0.7} 44-45°

Solubility: Sol. H₂O, EtOH, Me₂CO, CHCl₃

pKa Value: p*K*_a 9.96 (25°,H₂O)

Hazard & Toxicity: Severe eye and skin irritant. LD₅₀ (rbt, skn) 1250 mg/kg. Exp. teratogen. Fl. p. 80° (oc)

Aldrich: A7640-0

Fluka: 9290

Sigma: A0536

>>Derivative: O-Ac

Molecular Formula: C5H11NO2

Molecular Weight: 117.147

Accurate Mass: 117.078979

Percentage Composition: C 51.26%; H 9.46%; N 11.96%; O 27.31%

Melting Point: Mp 86° (as hydrochloride)

>>Derivative: O-Benzoyl

Molecular Formula: C10H13NO2

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Melting Point: Mp 182-183° (112°) (as hydrochloride)

>>Derivative: N-Benzoyl

Synonym(s): *N*-(3-Hydroxypropyl)benzamide

CAS Registry Number: 13609-09-1

Molecular Formula: C10H13NO2

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Physical Description: Needles (EtOAc)

Melting Point: Mp 60-60.5°

>>Derivative: Me ether

Synonym(s): 3-Methoxy-1-propylamine

CAS Registry Number: 5332-73-0

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: Bp 116°

pKa Value: p*K*_a 10.01 (25°,H₂O)

Aldrich: M2500-7

Fluka: 65309

Rare Chemicals Library: S42987-2