



>>Entry Name: 2-Amino-2-methylpropanoic acid, 9CI

Synonym(s): 2-Methylalanine, 8CI. α -Aminoisobutyric acid. Aib

CAS Registry Number: 62-57-7

$(\text{H}_3\text{C})_2\text{C}(\text{NH}_2)\text{COOH}$

Molecular Formula: $\text{C}_4\text{H}_9\text{NO}_2$

Molecular Weight: 103.121

Accurate Mass: 103.063329

Percentage Composition: C 46.59%; H 8.80%; N 13.58%; O 31.03%

Solubility: Spar. sol. EtOH; insol. Et₂O

pKa Value: $\text{p}K_{\text{a}1}$ 2.36; $\text{p}K_{\text{a}2}$ 10.21 (25°)

Other Data: Sublimes without melting at 280°

Aldrich: 85099-3

Fluka: 8280

Sigma: A8379

>>Derivative: Me ester

CAS Registry Number: 13257-67-5

Molecular Formula: $\text{C}_5\text{H}_{11}\text{NO}_2$

Molecular Weight: 117.147

Accurate Mass: 117.078979

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

Boiling Point: Bp 136°. Bp₂₀ 45°

>>Derivative: Me ester; hydrochloride

CAS Registry Number: 15028-41-8

Melting Point: Mp 186.5-187°

Solubility: Sol. H₂O, EtOH

Sigma: A8754

>>Derivative: Et ester

Molecular Formula: $\text{C}_6\text{H}_{13}\text{NO}_2$

Molecular Weight: 131.174

Accurate Mass: 131.094629

Percentage Composition: C 54.94%; H 9.99%; N 10.68%; O 24.39%

Physical Description: Cryst. (as hydrochloride)

Melting Point: Mp 159° (hydrochloride)

>>Derivative: Amide

CAS Registry Number: 16252-90-7

Molecular Formula: $\text{C}_4\text{H}_{10}\text{N}_2\text{O}$

Molecular Weight: 102.136

Accurate Mass: 102.079313

Percentage Composition: C 47.04%; H 9.87%; N 27.43%; O 15.66%

Physical Description: Cryst. (CHCl_3 /petrol)

Melting Point: Mp 127°

>>Derivative: Nitrile

Synonym(s): 2-Cyano-2-propylamine

CAS Registry Number: 19355-69-2

Molecular Formula: $\text{C}_4\text{H}_8\text{N}_2$

Molecular Weight: 84.121

Accurate Mass: 84.068748

Percentage Composition: C 57.11%; H 9.59%; N 33.30%

Physical Description: Oil

Boiling Point: Bp₁₅ 51-52°

Solubility: Sol. H₂O, EtOH, Et₂O, C₆H₆