>>**Entry Name: 2-Amino-2-methylpropanoic acid,** 9CI
**Synonym(s):** 2-Methylalanine, 8CI. α-Aminoisobutyric acid. Aib

**CAS Registry Number:** 62-57-7
$(H_3C)_2C(NH_2)COOH$

**Molecular Formula:** $C_4H_9NO_2$
**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. $Et_2O$
**pKa Value:** p$K_{a1}$ 2.36; p$K_{a2}$ 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:** $C_5H_{11}NO_2$
**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°. $Bp_{20}$ 45°

>>**Derivative:** Me ester; hydrochloride

**CAS Registry Number:** 15028-41-8
**Melting Point:** Mp 186.5-187°
**Solubility:** Sol. $H_2O$, EtOH
**Sigma:** A8754

>>**Derivative:** Et ester

**Molecular Formula:** $C_6H_{13}NO_2$
**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:** $C_4H_{10}N_2O$
**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:** $C_4H_8N_2$
**Molecular Weight:** 84.121
**Accurate Mass:** 84.068748
**Percentage Composition:** C 57.11%; H 9.59%; N 33.30%
**Physical Description:** Oil
**Boiling Point:** $Bp_{15}$ 51-52°
**Solubility:** Sol. $H_2O$, EtOH, $Et_2O$, $C_6H_6$

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