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>>Entry Name: 3-Aminopropanoic acid

Synonym(s):  $\beta$ -Alanine, 9CI. FEMA 3252

CAS Registry Number: 107-95-9

$\text{H}_2\text{NCH}_2\text{CH}_2\text{COOH}$

Molecular Formula:  $\text{C}_3\text{H}_7\text{NO}_2$

Molecular Weight: 89.094

Accurate Mass: 89.047679

Percentage Composition: C 40.44%; H 7.92%; N 15.72%; O 35.92%

Biological Source: Widely distributed in plants including algae, fungi and many higher plants. Residue present in Pantothenic acid [DGG30-H](#)

Use/Importance: Catalyst for Knoevenagel condensations. Used for synth. of Pantothenic acid [DGG30-H](#) and derivs.

Physical Description: Cryst. ( $\text{H}_2\text{O}$ )

Melting Point: Mp  $200^\circ$  (197-198 $^\circ$ )

Solubility: Sol.  $\text{H}_2\text{O}$ ; almost insol.  $\text{Et}_2\text{O}$ ,  $\text{Me}_2\text{CO}$

pKa Value:  $\text{p}K_{\text{a}1}$  3.7;  $\text{p}K_{\text{a}2}$  10.1 (30 $^\circ$ )

Aldrich: 23972-0

Fluka: 5160

Sigma: A7752

>>Derivative: Hydrochloride

CAS Registry Number: 6057-90-5

Physical Description: Plates

Melting Point: Mp  $123^\circ$

>>Derivative: Hydrobromide

CAS Registry Number: 30381-41-0

Physical Description: Needles

Melting Point: Mp 105-115 $^\circ$

>>Derivative: Me ester

CAS Registry Number: 4138-35-6

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%

Boiling Point:  $\text{Bp}_{15}$  58 $^\circ$

>>Derivative: Me ester; hydrochloride

CAS Registry Number: 3196-73-4

Physical Description: Scales

Melting Point: Mp 94-95 $^\circ$  (89-90 $^\circ$ )

Fluka: 5210

Sigma: A9515

>>Derivative: Et ester

CAS Registry Number: 924-73-2

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:  $\text{Bp}_{14}$  58 $^\circ$

>>Derivative: Et ester; hydrochloride

CAS Registry Number: 4244-84-2

Physical Description: Plates ( $\text{EtOH/Et}_2\text{O}$ )

Melting Point: Mp 69-70 $^\circ$

Aldrich: 30614-2

Fluka: 5182

Sigma: A2774