



>>Entry Name: 3-Amino-2,2-dimethylpropanoic acid, 9CI

Synonym(s): 2,2-Dimethyl-β-alanine, 8CI. Aminopivalic acid

CAS Registry Number: 19036-43-2

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

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%

Physical Description: Prisms (EtOH)

Melting Point: Mp 246°

>>Derivative: Me ester

CAS Registry Number: 25307-82-8

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: Deliquescent prisms (Et_2O)

Melting Point: Mp 64°

Boiling Point: Bp₁₁ 57°

>>Derivative: Me ester; hydrochloride

CAS Registry Number: 177269-37-3

Melting Point: Mp 164°

>>Derivative: Et ester

CAS Registry Number: 59193-77-0

Extra CAS Registry Numbers(s): 80253-38-9

Molecular Formula: $\text{C}_7\text{H}_{15}\text{NO}_2$

Molecular Weight: 145.201

Accurate Mass: 145.110279

Percentage Composition: C 57.90%; H 10.41%; N 9.65%; O 22.04%

Melting Point: Mp 91° (as hydrochloride)

>>Derivative: Amide

Molecular Formula: $\text{C}_5\text{H}_{12}\text{N}_2\text{O}$

Molecular Weight: 116.163

Accurate Mass: 116.094963

Percentage Composition: C 51.70%; H 10.41%; N 24.12%; O 13.77%

Physical Description: Cryst. (C_6H_6)

Melting Point: Mp 74-75°

>>Derivative: Nitrile

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

CAS Registry Number: 67744-70-1

Molecular Formula: $\text{C}_5\text{H}_{10}\text{N}_2$

Molecular Weight: 98.147

Accurate Mass: 98.084398

Percentage Composition: C 61.19%; H 10.27%; N 28.54%

Melting Point: Mp 10°

Boiling Point: Bp₁₅ 63°

>>Derivative: Lactam

References:

Buckley, G.D. *et al.*, *J.C.S.*, 1947, 1500-1503, (*synth*, *Me ester*, *amide*, *nitrile*)

Okano, K. *et al.*, *Chem. Pharm. Bull.*, 1985, **33**, 2228-2234, (*synth*, *pmr*, *cmr*)

Ducry, L. *et al.*, *Helv. Chim. Acta*, 1999, **82**, 2432-2447, (*synth*, *pmr*)