



>>Entry Name: **2,2-Dimethylpentanoic acid**, 9CI

Synonym(s): 2,2-Dimethylvaleric acid, 8CI

CAS Registry Number: 1185-39-3

H3CCH2CH2C(CH3)2COOH

Molecular Formula: C7H14O2

Molecular Weight: 130.186

Accurate Mass: 130.09938

Percentage Composition: C 64.58%; H 10.84%; O 24.58%

Physical Description: Liq.

Boiling Point: Bp₉ 98-99°

Density: d₄²⁰ 0.9189

Refractive Index: n_D²⁰ 1.4212

>>Derivative: Me ester

CAS Registry Number: 813-68-3

Molecular Formula: C8H16O2

Molecular Weight: 144.213

Accurate Mass: 144.11503

Percentage Composition: C 66.63%; H 11.18%; O 22.19%

Physical Description: Liq.

Boiling Point: Bp 144-145°

>>Derivative: Et ester

CAS Registry Number: 5837-93-4

Molecular Formula: C9H18O2

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Physical Description: Liq.

Boiling Point: Bp 161-161.5°

>>Derivative: Chloride

CAS Registry Number: 15721-22-9

Molecular Formula: C7H13ClO

Molecular Weight: 148.632

Accurate Mass: 148.065492

Percentage Composition: C 56.57%; H 8.82%; Cl 23.85%; O 10.76%

Physical Description: Liq.

Boiling Point: Bp₁₀ 45°

>>Derivative: Amide

CAS Registry Number: 13146-36-6

Molecular Formula: C7H15NO

Molecular Weight: 129.202

Accurate Mass: 129.115364

Percentage Composition: C 65.07%; H 11.70%; N 10.84%; O 12.38%

Melting Point: Mp 95-96°

>>Derivative: Nitrile

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

CAS Registry Number: 20654-47-1

Molecular Formula: C7H13N

Molecular Weight: 111.186

Accurate Mass: 111.104799

Percentage Composition: C 75.62%; H 11.78%; N 12.60%

Physical Description: Liq.

Boiling Point: Bp₄₀ 60°

References: