



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

Synonym(s): Pivalic acid, 8CI. Trimethylacetic acid. Neopentanoic acid

CAS Registry Number: 75-98-9

(H₃C)₃CCOOH

Molecular Formula: C₅H₁₀O₂

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

Melting Point: Mp 35.3-35.5°

Boiling Point: Bp 163.7-163.8°. Bp₂₀ 75-78°

pKa Value: pK_{a1} 5.04 (25°)

Hazard & Toxicity: LD₅₀ (rat,ori) 900 mg/kg

Aldrich: T7180-3

Fluka: 80882

Rare Chemicals Library: S37243-9

Sigma: P7407

>>Derivative: Me ester

CAS Registry Number: 598-98-1

Molecular Formula: C₆H₁₂O₂

Molecular Weight: 116.16

Accurate Mass: 116.08373

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Boiling Point: Bp 100-102°

Aldrich: M8650-2

Fluka: 80920

Sigma: P1532

>>Derivative: Et ester

CAS Registry Number: 3938-95-2

Molecular Formula: C₇H₁₄O₂

Molecular Weight: 130.186

Accurate Mass: 130.09938

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

Boiling Point: Bp 118°

Aldrich: 23455-9

Fluka: 80890

Rare Chemicals Library: S38546-8

Sigma: P6133

>>Derivative: 2,2-Dimethylpropyl ester

CAS Registry Number: 5340-26-1

Molecular Formula: C₁₀H₂₀O₂

Molecular Weight: 172.267

Accurate Mass: 172.14633

Percentage Composition: C 69.72%; H 11.70%; O 18.58%

Boiling Point: Bp 165°

Refractive Index: n_D²⁰ 1.4050

Aldrich: 33167-8

>>Derivative: Vinyl ester

Synonym(s): Vinyl pivalate

CAS Registry Number: 3377-92-2

Molecular Formula: C₇H₁₂O₂

Molecular Weight: 128.171

Accurate Mass: 128.08373

Percentage Composition: C 65.60%; H 9.44%; O 24.97%

Boiling Point: Bp 113-114°

Density: d₄²⁶ 0.88

Refractive Index: n_D²⁰ 1.4068