



>>Entry Name: 3,3-Dimethylpentanedioic acid, 9CI

Synonym(s): 3,3-Dimethylglutaric acid

CAS Registry Number: 4839-46-7

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

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}_4$

Molecular Weight: 160.169

Accurate Mass: 160.07356

Percentage Composition: C 52.49%; H 7.55%; O 39.96%

Physical Description: Needles (C_6H_6)

Melting Point: Mp 103-104°

Boiling Point: Bp₂ 89-90°

pKa Value: pK_{a1} 3.73; pK_{a2} 6.71 (25°)

Aldrich: D15940-9

Fluka: 40340

Sigma: D4379

>>Derivative: Mono-Me ester

CAS Registry Number: 27151-66-2

Molecular Formula: $\text{C}_8\text{H}_{14}\text{O}_4$

Molecular Weight: 174.196

Accurate Mass: 174.08921

Percentage Composition: C 55.16%; H 8.10%; O 36.74%

Boiling Point: Bp₆ 81°

>>Derivative: Mono-Me ester, chloride

CAS Registry Number: 61798-18-3

Molecular Formula: $\text{C}_8\text{H}_{13}\text{ClO}_3$

Molecular Weight: 192.642

Accurate Mass: 192.055322

Percentage Composition: C 49.88%; H 6.80%; Cl 18.40%; O 24.92%

Boiling Point: Bp₃ 75-76°

>>Derivative: Di-Me ester

CAS Registry Number: 19184-67-9

Molecular Formula: $\text{C}_9\text{H}_{16}\text{O}_4$

Molecular Weight: 188.223

Accurate Mass: 188.10486

Percentage Composition: C 57.43%; H 8.57%; O 34.00%

Boiling Point: Bp₁₅ 103-104°. Bp_{0.14} 70°

Rare Chemicals Library: S3497-6

>>Derivative: Dichloride

CAS Registry Number: 53120-75-5

Molecular Formula: $\text{C}_7\text{H}_{10}\text{Cl}_2\text{O}_2$

Molecular Weight: 197.06

Accurate Mass: 196.005784

Percentage Composition: C 42.67%; H 5.11%; Cl 35.98%; O 16.24%

Boiling Point: Bp₁₁ 95-96°

>>Derivative: Anhydride

Synonym(s): Dihydro-4,4-dimethyl-2H-pyran-2,6(3H)-dione

CAS Registry Number: 4160-82-1

Molecular Formula: $\text{C}_7\text{H}_{10}\text{O}_3$

Molecular Weight: 142.154

Accurate Mass: 142.062995

Percentage Composition: C 59.14%; H 7.09%; O 33.76%

Melting Point: Mp 124°

Aldrich: D15980-8