



>>Entry Name: 4,4-Dimethyl-3-oxopentanoic acid, 9CI

Synonym(s): 4,4-Dimethyl-3-oxovaleric acid, 8CI. (Trimethylacetyl)acetic acid

CAS Registry Number: 72531-41-0

Related CAS Registry Numbers(s): 32116-01-1 32265-87-5 54381-89-4 61540-31-6 77902-92-2

(H₃C)₃CCOCH₂COOH

Molecular Formula: C₇H₁₂O₃

Molecular Weight: 144.17

Accurate Mass: 144.078645

Percentage Composition: C 58.32%; H 8.39%; O 33.29%

Melting Point: Mp 47-49° (petrol or CHCl₃/pentane)

>>Derivative: Me ester

CAS Registry Number: 55107-14-7

Molecular Formula: C₈H₁₄O₃

Molecular Weight: 158.197

Accurate Mass: 158.094295

Percentage Composition: C 60.74%; H 8.92%; O 30.34%

Boiling Point: Bp₁₇ 82-84°. Bp₃ 68-73°

Aldrich: 26240-4

>>Derivative: Et ester

CAS Registry Number: 17094-34-7

Molecular Formula: C₉H₁₆O₃

Molecular Weight: 172.224

Accurate Mass: 172.109945

Percentage Composition: C 62.77%; H 9.36%; O 27.87%

Boiling Point: Bp₁₇ 82-84°

Density: d₄¹⁸ 0.97

Refractive Index: n_D²⁰ 1.4330

Fluka: 80940

Other: PB E14310

>>Derivative: Et ester, semicarbazone

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 117-117.5°

>>Derivative: Propyl ester

CAS Registry Number: 77067-73-3

Molecular Formula: C₁₀H₁₈O₃

Molecular Weight: 186.25

Accurate Mass: 186.125595

Percentage Composition: C 64.49%; H 9.74%; O 25.77%

Boiling Point: Bp₁₈ 109-111°

Refractive Index: n_D²⁰ 1.4331

>>Derivative: Amide

Molecular Formula: C₇H₁₃NO₂

Molecular Weight: 143.185

Accurate Mass: 143.094629

Percentage Composition: C 58.72%; H 9.15%; N 9.78%; O 22.35%

Physical Description: Plates (C₆H₆), cryst. (EtOAc/petrol)

Melting Point: Mp 95° (83-84°)