



>>Entry Name: 4-Oxoheptanedioic acid, 9CI

Synonym(s): Acetonediacetic acid. Hydrochelidonic acid.  $\gamma$ -Oxopimelic acid

CAS Registry Number: 502-50-1

$\text{CO}(\text{CH}_2\text{CH}_2\text{COOH})_2$

Molecular Formula:  $\text{C}_7\text{H}_{10}\text{O}_5$

Molecular Weight: 174.153

Accurate Mass: 174.052825

Percentage Composition: C 48.28%; H 5.79%; O 45.93%

Physical Description: Plates ( $\text{H}_2\text{O}$ )

Melting Point: Mp 139°

Other Data: Heat at Mp  $\rightarrow$  anhydride

Aldrich: K350-6

Fluka: 75939

Sigma: K3876

>>Derivative: Oxime

Molecular Formula:  $\text{C}_7\text{H}_{11}\text{NO}_5$

Molecular Weight: 189.168

Accurate Mass: 189.063724

Percentage Composition: C 44.45%; H 5.86%; N 7.40%; O 42.29%

Physical Description: Prisms ( $\text{H}_2\text{O}$ )

Melting Point: Mp 129 dec.°

>>Derivative: Semicarbazone

Melting Point: Mp 201-203 dec.°

>>Derivative: Di-Me ester

CAS Registry Number: 22634-92-0

Molecular Formula:  $\text{C}_9\text{H}_{14}\text{O}_5$

Molecular Weight: 202.207

Accurate Mass: 202.084125

Percentage Composition: C 53.46%; H 6.98%; O 39.56%

Physical Description: Needles ( $\text{EtOH}$ )

Melting Point: Mp 56°

Boiling Point: Bp 276-277° dec.

>>Derivative: Di-Me ester, oxime

Molecular Formula:  $\text{C}_9\text{H}_{15}\text{NO}_5$

Molecular Weight: 217.221

Accurate Mass: 217.095024

Percentage Composition: C 49.76%; H 6.96%; N 6.45%; O 36.83%

Physical Description: Needles ( $\text{CS}_2$ )

Melting Point: Mp 52°

>>Derivative: Mono-Et ester

CAS Registry Number: 1506-55-4

Molecular Formula:  $\text{C}_9\text{H}_{14}\text{O}_5$

Molecular Weight: 202.207

Accurate Mass: 202.084125

Percentage Composition: C 53.46%; H 6.98%; O 39.56%

Physical Description: Solid ( $\text{EtOAc}$ /hexane)

Melting Point: Mp 68.5-69.5°

>>Derivative: Di-Et ester

CAS Registry Number: 6317-49-3

Molecular Formula:  $\text{C}_{11}\text{H}_{18}\text{O}_5$

Molecular Weight: 230.26

Accurate Mass: 230.115425

Percentage Composition: C 57.38%; H 7.88%; O 34.74%

Boiling Point: Bp<sub>0.3</sub> 116-121°

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