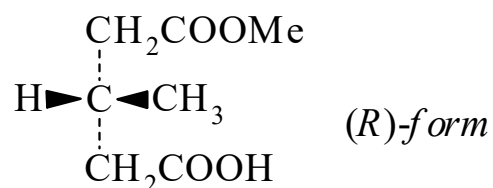




>>Entry Name: Monomethyl 3-methylpentanedioate, 9CI

Synonym(s): Monomethyl 3-methylglutarate, 9CI. Methyl hydrogen 3-methylglutarate



CAS Registry Number: 27151-65-1

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%

>>Variant: (R)-form

CAS Registry Number: 63473-60-9

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%

Use/Importance: Synthon for Kolbe electrolytic synth. of chiral long-chain branched carboxylic acids etc.

Boiling Point: $\text{Bp}_{0.4}$ 103-104.5°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +0.66$ (neat)

Aldrich: 38046-6

Fluka: 67024

>>Derivative: Et analogue

Synonym(s): Ethyl hydrogen 3-methylglutarate

CAS Registry Number: 72594-19-5

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%

Use/Importance: Synthon with similar uses to the Me ester

Optical Rotation: $[\alpha]_{\text{D}}^{25} -0.65$ (c, 5.6 in CH_3)

Fluka: 67000

>>Variant: (±)-form

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: Liq.

Boiling Point: Bp_1 114-116°

>>Derivative: Et analogue

Melting Point: Mp 144-146°

References:

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