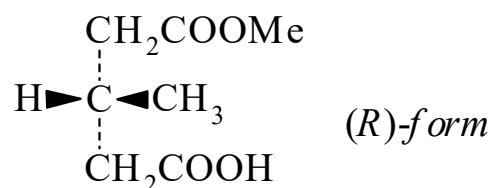




>>Entry Name: Monomethyl 3-methylpentanedioate, 9CI

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



CAS Registry Number: 27151-65-1

Molecular Formula: C₇H₁₂O₄

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: C₇H₁₂O₄

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: Bp_{0.4} 103-104.5°

Optical Rotation: [α]_D²⁵ +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: C₈H₁₄O₄

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: [α]_D²⁵ -0.65 (c, 5.6 in CH₃)

Fluka: 67000

>>Variant: (±)-form

Molecular Formula: C₇H₁₂O₄

Molecular Weight: 160.169

Accurate Mass: 160.07356

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

Physical Description: Liq.

Boiling Point: Bp₁ 114-116°

>>Derivative: Et analogue

Melting Point: Mp 144-146°

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 1119C, (*nmr*)
Ställberg-Stenhagen, S., *Ark. Kemi*, 1947, **25A**, no. 10; 1952, **3**, 117; 517, (*synth, resohn*)
Linstead, R.P. *et al.*, *J.C.S.*, 1950, 3333, (*synth*)
Mislow, K. *et al.*, *J.A.C.S.*, 1956, **78**, 5920, (*abs config*)
Holliday, I.A. *et al.*, *J.C.S.*, 1957, 2934, (*chloride*)
Conti, C. *et al.*, *Chim. Ind. (Milan)*, 1976, **58**, 877, (*synth*)
Mohr, P. *et al.*, *Helv. Chim. Acta*, 1982, **65**, 1412, (*synth, use*)
Alvarez, E. *et al.*, *Tetrahedron*, 1988, **44**, 119, (*synth, bibl*)
Andruszkiewicz, R. *et al.*, *Synth. Commun.*, 1990, **20**, 159, (*synth*)