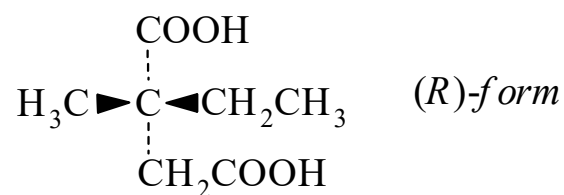




>>Entry Name: 2-Ethyl-2-methylbutanedioic acid, 9CI

Synonym(s): 2-Ethyl-2-methylsuccinic acid



CAS Registry Number: 631-31-2

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%

Aldrich: 15121-1

>>Variant: (R)-form

CAS Registry Number: 24410-76-2

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%

Optical Rotation: $[\alpha]_{\text{D}}^{22} +11.38$ (c, 5 in EtOH)

>>Variant: (S)-form

CAS Registry Number: 40710-02-9

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%

Optical Rotation: $[\alpha]_{\text{D}}^{22} -11.28$ (c, 5 in EtOH)

>>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: Prisms (H_2O)

Melting Point: Mp 104°

Boiling Point: Bp₁₂ $154\text{-}156^\circ$

pKa Value: pK_a 4.02

Other Data: Heat at $135^\circ \rightarrow$ anhydride

>>Derivative: 1-Me ester

CAS Registry Number: 43010-65-7

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%

Melting Point: Mp $35.8\text{-}36.3^\circ$

Boiling Point: Bp₁ $96\text{-}97^\circ$

>>Derivative: 4-Me ester

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%

Melting Point: Mp $71.9\text{-}72.4^\circ$

Boiling Point: Bp_{0.2} $93\text{-}94^\circ$