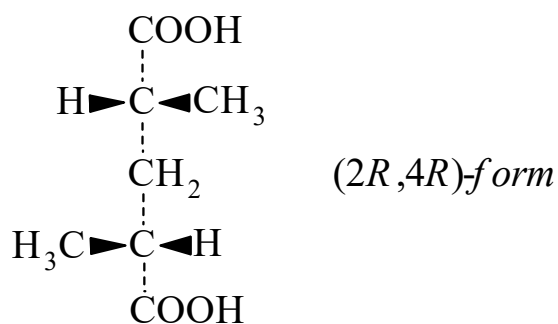




>>Entry Name: 2,4-Dimethylpentanedioic acid, 9CI

Synonym(s): 2,4-Dimethylglutaric acid



CAS Registry Number: 2121-67-7

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: (2R,4R)-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: Needles (H_2O)

Melting Point: Mp 79.5-80°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -39.8$ (H_2O)

>>Derivative: Anhydride

Molecular Formula: $\text{C}_7\text{H}_{10}\text{O}_3$

Molecular Weight: 142.154

Accurate Mass: 142.062995

Percentage Composition: C 59.14%; H 7.09%; O 33.76%

Melting Point: Mp 41.5-42.5°

Optical Rotation: $[\alpha]_{\text{D}}^{18} -69.6$ (C_6H_6)

>>Variant: (2S,4S)-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%

Melting Point: Mp 79-80°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +39.8$ (H_2O)

>>Derivative: Anhydride

Melting Point: Mp 41.5-42.5°

Optical Rotation: $[\alpha]_{\text{D}} +69.6$ (C_6H_6)

>>Variant: (2RS,3RS)-form

Synonym(s): ($\pm$)-form

CAS Registry Number: 3891-69-8

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

Melting Point: Mp 143-145°

pKa Value: $\text{p}K_{\text{a}1}$ 4.24; $\text{p}K_{\text{a}2}$ 5.82

Other Data: Steam-volatile