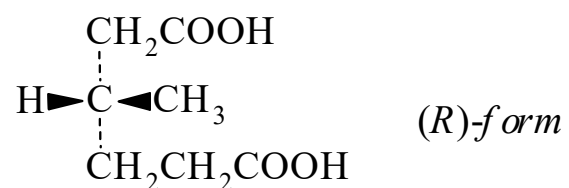




>>Entry Name: 3-Methylhexanedioic acid, 9CI, 8CI

Synonym(s): 2-Methylbutane-1,4-dicarboxylic acid. 3-Methyladipic acid



CAS Registry Number: 3058-01-3

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: M2740-9

Sigma: M5137

>>Variant: (R)-form

CAS Registry Number: 623-82-5

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: Comonomer in liq. cryst. polyesters

Physical Description: Cryst. (C_6H_6)

Melting Point: Mp 93-94.5°

Boiling Point: Bp₃₀ 230°. Bp₈ 205°

Optical Rotation: $[\alpha]_{\text{D}}^{26} +11.67$ (c, 1.2 in CHCl_3) (100% ee)

Solubility: Sol. H_2O , EtOH, CHCl_3 , EtOAc

Aldrich: 36891-1

Fluka: 65510

>>Derivative: 6-Mono-Et ester

Molecular Formula: $\text{C}_9\text{H}_{16}\text{O}_4$

Molecular Weight: 188.223

Accurate Mass: 188.10486

Percentage Composition: C 57.43%; H 8.57%; O 34.00%

Boiling Point: Bp₁₁ 164-166°

>>Derivative: Di-Et ester

Molecular Formula: $\text{C}_{11}\text{H}_{20}\text{O}_4$

Molecular Weight: 216.277

Accurate Mass: 216.13616

Percentage Composition: C 61.09%; H 9.32%; O 29.59%

Boiling Point: Bp₇₄₆ 257°. Bp₁₀ 126.5°

>>Derivative: Dichloride

Molecular Formula: $\text{C}_7\text{H}_{10}\text{Cl}_2\text{O}_2$

Molecular Weight: 197.06

Accurate Mass: 196.005784

Percentage Composition: C 42.67%; H 5.11%; Cl 35.98%; O 16.24%

Boiling Point: Bp₁₀ 117-119°

>>Derivative: Diamide

Molecular Formula: $\text{C}_7\text{H}_{14}\text{N}_2\text{O}_2$

Molecular Weight: 158.2

Accurate Mass: 158.105528

Percentage Composition: C 53.15%; H 8.92%; N 17.71%; O 20.23%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 191°

Solubility: Sol. H_2O ; insol. Et_2O