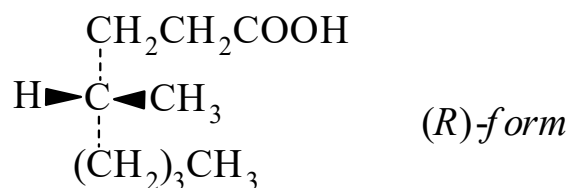




>>Entry Name: 4-Methyloctanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 4-Methylcaprylic acid. FEMA 3575



CAS Registry Number: 54947-74-9

Molecular Formula: C₉H₁₈O₂

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Aldrich: W35750-2

Sigma: M7400

>>Variant: (R)-form

Molecular Formula: C₉H₁₈O₂

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Boiling Point: Bp₂₅ 166-172°

Optical Rotation: [α]_D −1.53 (c, 1.114 in CHCl₃) (ca. 95% ee)

>>Variant: (S)-form

Molecular Formula: C₉H₁₈O₂

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Optical Rotation: [α]_D +1.45 (c, 1.106 in CHCl₃) (ca. 95% ee)

>>Variant: (±)-form

Molecular Formula: C₉H₁₈O₂

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Use/Importance: Flavouring ingredient

Boiling Point: Bp₁₀ 140-142°. Bp₂ 110.5-111.5°

Density: d²⁰ 0.91

Refractive Index: n_D²⁰ 1.4335

>>Derivative: S-Benzylthiouronium salt

Physical Description: Needles

Melting Point: Mp 135°

>>Derivative: Et ester

CAS Registry Number: 56196-53-3

Molecular Formula: C₁₁H₂₂O₂

Molecular Weight: 186.294

Accurate Mass: 186.16198

Percentage Composition: C 70.92%; H 11.90%; O 17.18%

Biological Source: Aggregation pheromone of the male beetle *Oryctes monoceros*

Boiling Point: Bp₇ 140°. Bp₂ 108°

References: