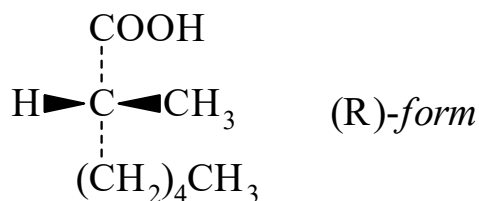




>>Entry Name: 2-Methylheptanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Amylmethylacetic acid. FEMA 2706



CAS Registry Number: 1188-02-9

Related CAS Registry Numbers(s): 13751-83-2

Molecular Formula: C₈H₁₆O₂

Molecular Weight: 144.213

Accurate Mass: 144.11503

Percentage Composition: C 66.63%; H 11.18%; O 22.19%

Aldrich: W27060-1

>>Variant: (R)-form

CAS Registry Number: 159345-59-2

Molecular Formula: C₈H₁₆O₂

Molecular Weight: 144.213

Accurate Mass: 144.11503

Percentage Composition: C 66.63%; H 11.18%; O 22.19%

Physical Description: Liq.

Boiling Point: Bp₁₃ 121-122°

Optical Rotation: [α]_D²⁵ -15.6 (neat) (86% ee)

>>Derivative: Chloride

Molecular Formula: C₈H₁₅ClO

Molecular Weight: 162.659

Accurate Mass: 162.081142

Percentage Composition: C 59.07%; H 9.29%; Cl 21.80%; O 9.84%

Physical Description: Liq.

Boiling Point: Bp₇₂₇ 179.5-182°

>>Variant: (S)-form

CAS Registry Number: 116454-37-6

Molecular Formula: C₈H₁₆O₂

Molecular Weight: 144.213

Accurate Mass: 144.11503

Percentage Composition: C 66.63%; H 11.18%; O 22.19%

Optical Rotation: [α]_D²⁰ +4.1 (neat)

>>Variant: (±)-form

CAS Registry Number: 128441-06-5

Molecular Formula: C₈H₁₆O₂

Molecular Weight: 144.213

Accurate Mass: 144.11503

Percentage Composition: C 66.63%; H 11.18%; O 22.19%

Use/Importance: Flavouring ingredient

Melting Point: Mp 15°

Boiling Point: Bp₁₃ 121-122°

References: