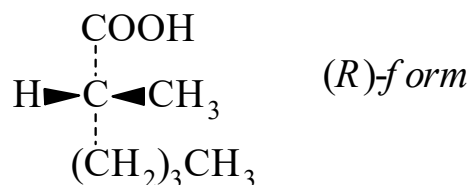




>>Entry Name: 2-Methylhexanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2-Methylcaproic acid. Hexane-2-carboxylic acid. FEMA 3191



CAS Registry Number: 4536-23-6

Molecular Formula: C₇H₁₄O₂

Molecular Weight: 130.186

Accurate Mass: 130.09938

Percentage Composition: C 64.58%; H 10.84%; O 24.58%

Aldrich: 33827-3

Fluka: 67435

>>Variant: (R)-form

CAS Registry Number: 51703-97-0

Molecular Formula: C₇H₁₄O₂

Molecular Weight: 130.186

Accurate Mass: 130.09938

Percentage Composition: C 64.58%; H 10.84%; O 24.58%

Physical Description: Oil

Boiling Point: Bp₅ 105°

Optical Rotation: [α]_D²⁰ -24.3 (neat). [α]_D²⁰ -19.7 (c, 0.5 in CH₂Cl₂)

>>Derivative: 4-Nitrophenyl ester

Boiling Point: Bp_{0.01} 138°

Optical Rotation: [α]_D -55 (heptane). [α]_D -148 (neat)

>>Variant: (S)-form

CAS Registry Number: 49642-51-5

Molecular Formula: C₇H₁₄O₂

Molecular Weight: 130.186

Accurate Mass: 130.09938

Percentage Composition: C 64.58%; H 10.84%; O 24.58%

Physical Description: Oil

Boiling Point: Bp₅ 105°

Optical Rotation: [α]_D²⁹ +19 (neat)

>>Variant: (±)-form

CAS Registry Number: 22160-12-9

Molecular Formula: C₇H₁₄O₂

Molecular Weight: 130.186

Accurate Mass: 130.09938

Percentage Composition: C 64.58%; H 10.84%; O 24.58%

Use/Importance: Flavouring ingredient

Physical Description: Oil

Boiling Point: Bp 215-216°. Bp₅ 72°

Density: d₄²⁰ 0.961

pKa Value: pK_a 5.04 (0.1M KCl)

Refractive Index: n_D²⁰ 1.4193

>>Derivative: Me ester