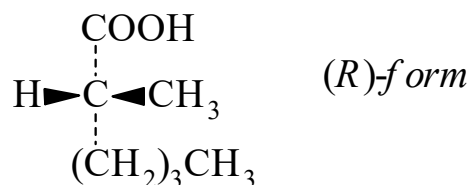




>>Entry Name: 2-Methylhexanoic acid, 9CI

ENTRY UNDER REVIEW

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



CAS Registry Number: 4536-23-6

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

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

Molecular Weight: 130.186

Accurate Mass: 130.09938

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

Physical Description: Oil

Boiling Point: Bp_5 105°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -24.3$ (neat). $[\alpha]_{\text{D}}^{20} -19.7$ (c, 0.5 in CH_2Cl_2)

>>Derivative: 4-Nitrophenyl ester

Boiling Point: $\text{Bp}_{0.01}$ 138°

Optical Rotation: $[\alpha]_{\text{D}} -55$ (heptane). $[\alpha]_{\text{D}} -148$ (neat)

>>Variant: (S)-form

CAS Registry Number: 49642-51-5

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

Molecular Weight: 130.186

Accurate Mass: 130.09938

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

Physical Description: Oil

Boiling Point: Bp_5 105°

Optical Rotation: $[\alpha]_{\text{D}}^{29} +19$ (neat)

>>Variant: (±)-form

CAS Registry Number: 22160-12-9

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

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°. Bp_5 72°

Density: d_4^{20} 0.961

pKa Value: pK_a 5.04 (0.1M KCl)

Refractive Index: n_{D}^{20} 1.4193

>>Derivative: Me ester