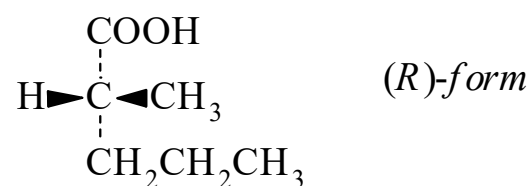




>>Entry Name: 2-Methylpentanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2-Methylvaleric acid. FEMA 2754



CAS Registry Number: 97-61-0

Related CAS Registry Numbers(s): 6339-13-5

Molecular Formula: C₆H₁₂O₂

Molecular Weight: 116.16

Accurate Mass: 116.08373

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Hazard & Toxicity: Fl.p. 107° (oc), autoignition temp. 378°. Skin and eye irritant. LD₅₀ (rat, orl) 2040 mg/kg

Aldrich: W27540-9

Rare Chemicals Library: S44207-0

>>Variant: (R)-form

CAS Registry Number: 49642-47-9

Molecular Formula: C₆H₁₂O₂

Molecular Weight: 116.16

Accurate Mass: 116.08373

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Boiling Point: Bp₁₅ 96°

Optical Rotation: [α]_D −18.4 (neat)

>>Derivative: Et ester

CAS Registry Number: 151526-65-7

Molecular Formula: C₈H₁₆O₂

Molecular Weight: 144.213

Accurate Mass: 144.11503

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

Boiling Point: Bp₄ 78-80°

Optical Rotation: [α]_D²⁵ −7.91

>>Derivative: Amide

CAS Registry Number: 34241-21-9

Molecular Formula: C₆H₁₃NO

Molecular Weight: 115.175

Accurate Mass: 115.099714

Percentage Composition: C 62.57%; H 11.38%; N 12.16%; O 13.89%

Melting Point: Mp 78°

Optical Rotation: [α]_D²⁵ −5.79 (EtOH aq.)

>>Derivative: Nitrile

Synonym(s): 2-Cyanopentane

Molecular Formula: C₆H₁₁N

Molecular Weight: 97.16

Accurate Mass: 97.089149

Percentage Composition: C 74.17%; H 11.41%; N 14.42%

Boiling Point: Bp₂ 30-32°

Optical Rotation: [α]_D²⁵ −13.77

>>Variant: (S)-form

CAS Registry Number: 1187-82-2