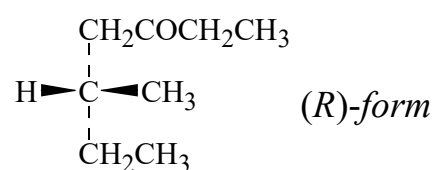




>>Entry Name: 5-Methyl-3-heptanone, 9CI



CAS Registry Number: 541-85-5

Extra CAS Registry Numbers(s): 116003-10-2

Molecular Formula: C₈H₁₆O

Molecular Weight: 128.214

Accurate Mass: 128.120115

Percentage Composition: C 74.94%; H 12.58%; O 12.48%

Hazard & Toxicity: Flammable. Skin and eye irritant. OES: long-term 25 ppm

Aldrich: 10940-1

Fluka: 67260

Rare Chemicals Library: S41184-1

>>Variant: (R)-form

CAS Registry Number: 116003-10-2

Molecular Formula: C₈H₁₆O

Molecular Weight: 128.214

Accurate Mass: 128.120115

Percentage Composition: C 74.94%; H 12.58%; O 12.48%

Biological Source: Sex pheromone of male *Platynereis dumerilii*.

Boiling Point: Bp₄₀ 100°

Optical Rotation: [α]_D²⁰+5.31 (c, 4.20 in C₆H₆) (>=98% ee). [α]_D²⁰-8.73 (neat)

>>Variant: (S)-form

CAS Registry Number: 20616-93-7

Molecular Formula: C₈H₁₆O

Molecular Weight: 128.214

Accurate Mass: 128.120115

Percentage Composition: C 74.94%; H 12.58%; O 12.48%

Biological Source: Sex pheromone of female *Platynereis dumerilii*.

Boiling Point: Bp₁₆ 54-55°

Optical Rotation: [α]_D²⁵+8.57 (neat)

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Cryst. (EtOH)

Melting Point: Mp 66-67°

>>Variant: (±)-form

CAS Registry Number: 57968-70-4

Molecular Formula: C₈H₁₆O

Molecular Weight: 128.214

Accurate Mass: 128.120115

Percentage Composition: C 74.94%; H 12.58%; O 12.48%

Physical Description: Liq. with minty odour

Boiling Point: Bp 161°

>>Derivative: Oxime