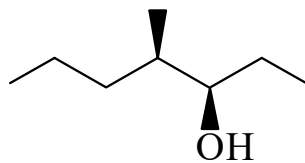




>>Entry Name: 4-Methyl-3-heptanol, 9CI



(3*R*,4*R*)-form

CAS Registry Number: 14979-39-6

Related CAS Registry Numbers(s): 63707-89-1 63707-90-4 73177-00-1 73177-01-2

Molecular Formula: C₈H₁₈O

Molecular Weight: 130.23

Accurate Mass: 130.135765

Percentage Composition: C 73.78%; H 13.93%; O 12.29%

Aldrich: M4830-9

>>Variant: (3*R*,4*R*)-form

CAS Registry Number: 63730-39-2

Molecular Formula: C₈H₁₈O

Molecular Weight: 130.23

Accurate Mass: 130.135765

Percentage Composition: C 73.78%; H 13.93%; O 12.29%

Physical Description: Liq.

Optical Rotation: $[\alpha]_{\text{D}}^{23} +21$ (hexane)

>>Variant: (3*R*,4*S*)-form

CAS Registry Number: 68509-47-7

Molecular Formula: C₈H₁₈O

Molecular Weight: 130.23

Accurate Mass: 130.135765

Percentage Composition: C 73.78%; H 13.93%; O 12.29%

Biological Source: Identified in the poison gland of *Leptogenys diminuta*

Optical Rotation: $[\alpha]_{\text{D}}^{25} -12$ (hexane)

>>Variant: (3*S*,4*R*)-form

CAS Registry Number: 63782-91-2

Molecular Formula: C₈H₁₈O

Molecular Weight: 130.23

Accurate Mass: 130.135765

Percentage Composition: C 73.78%; H 13.93%; O 12.29%

Biological Source: A pheromone of the smaller European bark beetle

Physical Description: Liq.

Boiling Point: Bp 160-161°. Bp₁₁₈ 105-115°

Optical Rotation: $[\alpha]_{\text{D}} +11.8$ (c, 1.9 in hexane)

>>Variant: (3*S*,4*S*)-form

CAS Registry Number: 68509-48-8

Molecular Formula: C₈H₁₈O

Molecular Weight: 130.23

Accurate Mass: 130.135765

Percentage Composition: C 73.78%; H 13.93%; O 12.29%

Biological Source: Component of the aggregation pheromone of the smaller European elm bark beetle *Scolytus multistriatus*

Physical Description: Volatile liq.

Optical Rotation: $[\alpha]_{\text{D}} -23.3$ (c, 1 in hexane)

References: