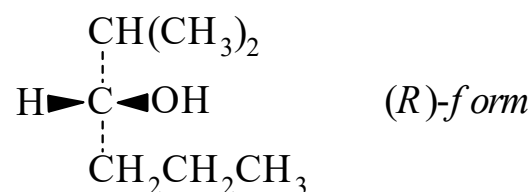




>>Entry Name: 2-Methyl-3-hexanol, 9CI

Synonym(s): Isopropylpropylcarbinol



CAS Registry Number: 617-29-8

Related CAS Registry Numbers(s): 61184-92-7

Molecular Formula: C₇H₁₆O

Molecular Weight: 116.203

Accurate Mass: 116.120115

Percentage Composition: C 72.35%; H 13.88%; O 13.77%

Aldrich: M4983-6

>>Variant: (R)-form

CAS Registry Number: 90670-72-7

Molecular Formula: C₇H₁₆O

Molecular Weight: 116.203

Accurate Mass: 116.120115

Percentage Composition: C 72.35%; H 13.88%; O 13.77%

Boiling Point: Bp 145-146°

Optical Rotation: [α]_D²⁰ +23.34 (c, 4.97 in CHCl₃)

>>Derivative: Hydrogen phthalate

Melting Point: Mp 79-80°

Optical Rotation: [α]_D +8.36 (EtOH)

>>Variant: (±)-form

CAS Registry Number: 100295-82-7

Molecular Formula: C₇H₁₆O

Molecular Weight: 116.203

Accurate Mass: 116.120115

Percentage Composition: C 72.35%; H 13.88%; O 13.77%

Boiling Point: Bp 141-142°

Solubility: Insol. H₂O

>>Derivative: Ac

Molecular Formula: C₉H₁₈O₂

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Boiling Point: Bp 164-166°

>>Derivative: 3,5-Dinitrobenzoyl

Melting Point: Mp 59-60°

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