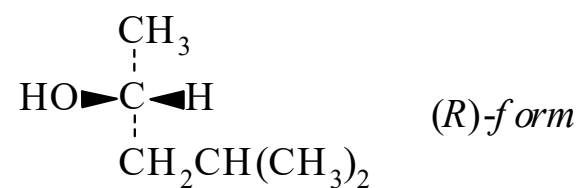




>>Entry Name: 4-Methyl-2-pentanol, 9CI

Synonym(s): Isobutylmethylcarbinol



Molecular Formula: C₆H₁₄O

Molecular Weight: 102.176

Accurate Mass: 102.104465

Percentage Composition: C 70.53%; H 13.81%; O 15.66%

>>Variant: (R)-form

CAS Registry Number: 16404-54-9

Molecular Formula: C₆H₁₄O

Molecular Weight: 102.176

Accurate Mass: 102.104465

Percentage Composition: C 70.53%; H 13.81%; O 15.66%

Physical Description: Liq.

Boiling Point: Bp₄₅ 64-65°

Optical Rotation: [α]_D²⁰ -20.8 (neat)

>>Derivative: 1-Naphthylurethane

Melting Point: Mp 86-89°

Optical Rotation: [α]_D²² -3.7 (EtOH)

>>Variant: (S)-form

CAS Registry Number: 14898-80-7

Molecular Formula: C₆H₁₄O

Molecular Weight: 102.176

Accurate Mass: 102.104465

Percentage Composition: C 70.53%; H 13.81%; O 15.66%

Physical Description: Liq.

Boiling Point: Bp₄₅ 63-64°

Optical Rotation: [α]_D²⁰ +22.4 (neat)

>>Variant: (±)-form

CAS Registry Number: 108-11-2

Molecular Formula: C₆H₁₄O

Molecular Weight: 102.176

Accurate Mass: 102.104465

Percentage Composition: C 70.53%; H 13.81%; O 15.66%

Physical Description: Liq.

Boiling Point: Bp 132°. Bp₁₀ 47°

Hazard & Toxicity: Flammable, fl. p. 41°. High vapour conc. anaesthetic. Skin and severe eye irritant. LD₅₀ (rat, orl) 2590 mg/kg. OES: long-term 25 ppm; short-term 40 ppm (Sk)

Aldrich: 10991-6

Fluka: 68440

>>Derivative: Phenylurethane

Melting Point: Mp 143°

>>Derivative: Ac