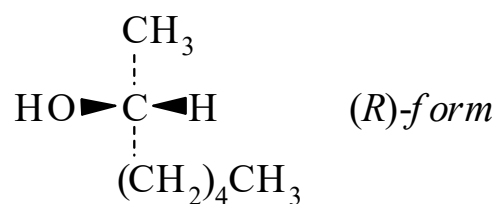




>>Entry Name: 2-Heptanol, 9CI

ENTRY UNDER REVIEW

Synonym(s): 1-Methylhexanol. FEMA 3288



CAS Registry Number: 543-49-7

Related CAS Registry Numbers(s): 5921-82-4 54638-12-9

Extra CAS Registry Numbers(s): 53535-33-4

Molecular Formula: C₇H₁₆O

Molecular Weight: 116.203

Accurate Mass: 116.120115

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

Biological Source: Occurs in oils of *Zingiber officinale*, *Fragaria vesca*, *Catharanthus roseus*. Released by *Curvularia falcata* and *Mucor* spp.

Hazard & Toxicity: Eye and skin irritant. LD₅₀ (rat,orl) 2580 mg/kg. Fl. p. 71°

Aldrich: W32880-4

Fluka: 51800

Supelco: 44-2351

>>Variant: (R)-form

CAS Registry Number: 6033-24-5

Molecular Formula: C₇H₁₆O

Molecular Weight: 116.203

Accurate Mass: 116.120115

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

Boiling Point: Bp₂₃ 74.5°

Optical Rotation: [α]_D²⁵ -3.78 (neat)

Aldrich: 40869-7

Sigma: H5649

>>Variant: (S)-form

CAS Registry Number: 6033-23-4

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 150°. Bp₂₀ 73.5°

Optical Rotation: [α]_D²⁵ +4.12 (neat). [α]_D²⁰ +11.45 (EtOH)

Aldrich: 34033-2

Rare Chemicals Library: S40609-0

>>Derivative: O-β-D-Glucopyranoside

CAS Registry Number: 117074-18-7

Molecular Formula: C₁₃H₂₆O₆

Molecular Weight: 278.345

Accurate Mass: 278.17294

Percentage Composition: C 56.10%; H 9.41%; O 34.49%

Biological Source: Constit. of *Lessingia glandulifera*

>>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: Bp₁₇ 71°

Optical Rotation: [α]_D²⁰ +8.23