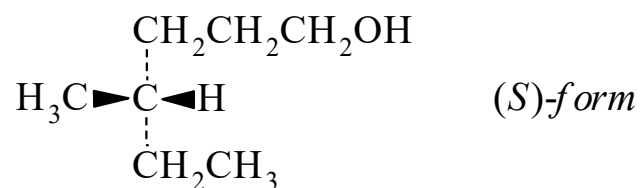




>>Entry Name: 4-Methyl-1-hexanol, 9CI



CAS Registry Number: 818-49-5

Related CAS Registry Numbers(s): 53353-04-1

Molecular Formula: C₇H₁₆O

Molecular Weight: 116.203

Accurate Mass: 116.120115

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

Biological Source: Isol. from the flowers of *Nicotiana sylvestris*

>>Variant: (S)-form

CAS Registry Number: 1767-46-0

Molecular Formula: C₇H₁₆O

Molecular Weight: 116.203

Accurate Mass: 116.120115

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

Boiling Point: Bp₁₄₀ 126°

Optical Rotation: [α]_D²⁵ +7.55 (neat). [α]_D²³ +8.62 (c, 3.65 in CHCl₃)

>>Variant: (±)-form

CAS Registry Number: 111768-05-9

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 173°. Bp₂₃ 83°

Density: d₂₀²⁰ 0.824

Refractive Index: n_D²⁰ 1.4219

>>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 190°

>>Derivative: 1-Naphthylurethane

Melting Point: Mp 50°

References:

- Cason, J. *et al.*, *J.O.C.*, 1948, **13**, 239-248, (*synth*)
Lardicci, L. *et al.*, *Gazz. Chim. Ital.*, 1961, **91**, 428-440; 441-457, (*synth*)
Julia, M. *et al.*, *Bull. Soc. Chim. Fr.*, 1964, 2533-2541; 3207-3217, (*synth*)
Carlini, C. *et al.*, *Gazz. Chim. Ital.*, 1973, **103**, 1297-1301, (*synth*)
Mori, K. *et al.*, *Tetrahedron*, 1978, **34**, 3119-3123; 1982, **38**, 2291-2297, (*synth, ir, pmr*)
Kandra, L. *et al.*, *Phytochemistry*, 1998, **49**, 1599-1604, (*isol, biosynth*)
Larsson, M. *et al.*, *Eur. J. Org. Chem.*, 2001, 353-363, (*S-form, synth, pmr, cmr, ms*)