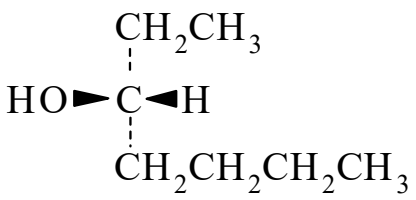
>>**Entry Name: 3-Heptanol,** 9CI
ENTRY UNDER REVIEW
Synonym(s): FEMA 3547



(*R*)-*form*

CAS Registry Number: 589-82-2
Extra CAS Registry Numbers(s): 53535-33-4

Molecular Formula: $C_7H_{16}O$
Molecular Weight: 116.203
Accurate Mass: 116.120115
Percentage Composition: C 72.35%; H 13.88%; O 13.77%
Biological Source: Present in strawberry, mint and banana
Use/Importance: Flavouring agent
Hazard & Toxicity: Eye and skin irritant. LD_{50} (rat,orl) 1870 mg/kg. Fl. p. 60°

Aldrich: W35470-8
Fluka: 51820

>>**Variant:** (*R*)-form

CAS Registry Number: 62701-49-9
Molecular Formula: $C_7H_{16}O$
Molecular Weight: 116.203
Accurate Mass: 116.120115
Percentage Composition: C 72.35%; H 13.88%; O 13.77%
Boiling Point: Bp_{18} 66°
Optical Rotation: $[\alpha]_D^{23}$ –0.9

>>**Derivative:** α-Naphthylurethane

Melting Point: Mp 74-75°
Optical Rotation: $[\alpha]_D^{20}$ 0

>>**Variant:** (*S*)-form

CAS Registry Number: 26549-25-7
Molecular Formula: $C_7H_{16}O$
Molecular Weight: 116.203
Accurate Mass: 116.120115
Percentage Composition: C 72.35%; H 13.88%; O 13.77%
Boiling Point: Bp_{117} 104-106°. Bp_{18} 66°

>>**Variant:** (±)-form

CAS Registry Number: 40617-58-1
Molecular Formula: $C_7H_{16}O$
Molecular Weight: 116.203
Accurate Mass: 116.120115
Percentage Composition: C 72.35%; H 13.88%; O 13.77%
Physical Description: Oily liq. with a powerful herbaceous odour and a pungent taste
Boiling Point: Bp_{750} 156.5-157°
Solubility: Isol. H_2O, Sol. EtOH

>>**Derivative:** Et ether
Synonym(s): 3-Ethoxyheptane

Molecular Formula: $C_9H_{20}O$
Molecular Weight: 144.256
Accurate Mass: 144.151415
Percentage Composition: C 74.94%; H 13.97%; O 11.09%
Boiling Point: Bp_{750} 151°

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