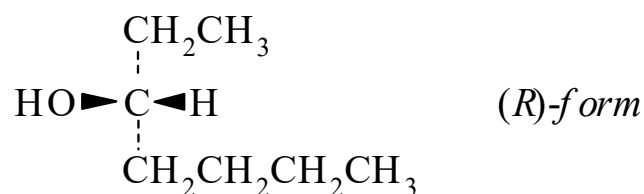




>>Entry Name: 3-Heptanol, 9CI

ENTRY UNDER REVIEW

Synonym(s): FEMA 3547



CAS Registry Number: 589-82-2

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: Present in strawberry, mint and banana

Use/Importance: Flavouring agent

Hazard & Toxicity: Eye and skin irritant. LD₅₀ (rat,orl) 1870 mg/kg. Fl. p. 60°

Aldrich: W35470-8

Fluka: 51820

>>Variant: (R)-form

CAS Registry Number: 62701-49-9

Molecular Formula: C₇H₁₆O

Molecular Weight: 116.203

Accurate Mass: 116.120115

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

Boiling Point: Bp₁₈ 66°

Optical Rotation: [α]_D²³ -0.9

>>Derivative: α-Naphthylurethane

Melting Point: Mp 74-75°

Optical Rotation: [α]_D²⁰ 0

>>Variant: (S)-form

CAS Registry Number: 26549-25-7

Molecular Formula: C₇H₁₆O

Molecular Weight: 116.203

Accurate Mass: 116.120115

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

Boiling Point: Bp₁₁₇ 104-106°. Bp₁₈ 66°

>>Variant: (±)-form

CAS Registry Number: 40617-58-1

Molecular Formula: C₇H₁₆O

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: Bp₇₅₀ 156.5-157°

Solubility: Isol. H₂O, Sol. EtOH

>>Derivative: Et ether

Synonym(s): 3-Ethoxyheptane

Molecular Formula: C₉H₂₀O

Molecular Weight: 144.256

Accurate Mass: 144.151415

Percentage Composition: C 74.94%; H 13.97%; O 11.09%

Boiling Point: Bp₇₅₀ 151°