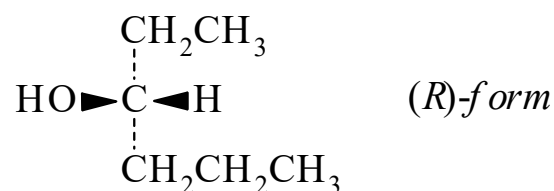




>>Entry Name: 3-Hexanol, 9CI

ENTRY UNDER REVIEW

Synonym(s): FEMA 3351



CAS Registry Number: 623-37-0

Related CAS Registry Numbers(s): 66585-24-8 66585-38-4

Extra CAS Registry Numbers(s): 25917-35-5

Molecular Formula: C₆H₁₄O

Molecular Weight: 102.176

Accurate Mass: 102.104465

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

Aldrich: W33511-8

Fluka: 52860

>>Variant: (R)-form

CAS Registry Number: 13471-42-6

Molecular Formula: C₆H₁₄O

Molecular Weight: 102.176

Accurate Mass: 102.104465

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

Boiling Point: Bp 133-134°

Optical Rotation: $[\alpha]_{\text{Hg}^{20}}^{20} -7.13$

>>Variant: (S)-form

CAS Registry Number: 6210-51-1

Molecular Formula: C₆H₁₄O

Molecular Weight: 102.176

Accurate Mass: 102.104465

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

Boiling Point: Bp 131-133°

Optical Rotation: $[\alpha]_{\text{Hg}^{20}}^{20} +6.81$ (CHCl₃)

>>Variant: (±)-form

CAS Registry Number: 17015-11-1

Molecular Formula: C₆H₁₄O

Molecular Weight: 102.176

Accurate Mass: 102.104465

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

Use/Importance: Flavouring ingredient

Boiling Point: Bp 134.5-135.5°

Solubility: Sl. sol. H₂O, sol. EtOH, Me₂CO, Et₂O

Density: d₂₀²⁰ 0.82

Refractive Index: n_D²⁰ 1.4167

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