



>>Entry Name: 3-Hexen-1-ol, 9CI

ENTRY UNDER REVIEW

Synonym(s): 3-Hexenyl alcohol. Leaf alcohol

CAS Registry Number: 544-12-7

Related CAS Registry Numbers(s): 53398-84-8

$\text{H}_3\text{CCH}_2\text{CH}=\text{CHCH}_2\text{CH}_2\text{OH}$

Molecular Formula: $\text{C}_6\text{H}_{12}\text{O}$

Molecular Weight: 100.16

Accurate Mass: 100.088815

Percentage Composition: C 71.95%; H 12.08%; O 15.97%

>>Variant: (*E*)-form

CAS Registry Number: 928-97-2

Molecular Formula: $\text{C}_6\text{H}_{12}\text{O}$

Molecular Weight: 100.16

Accurate Mass: 100.088815

Percentage Composition: C 71.95%; H 12.08%; O 15.97%

Use/Importance: Used in blueberry flavouring

Boiling Point: Bp 153-156°. Bp₂₂ 80-85°. Bp₂₀ 72.5-73°

Aldrich: W50780-6

Fluka: 53058

>>Derivative: 3,5-Dinitrobenzoyl

Melting Point: Mp 49°. Mp 46.5-47.3°

>>Derivative: 4-Nitrophenylurethane

Melting Point: Mp 84-85°

>>Variant: (*Z*)-form

Synonym(s): Phyllol. Verdolol. FEMA 2563

CAS Registry Number: 928-96-1

Molecular Formula: $\text{C}_6\text{H}_{12}\text{O}$

Molecular Weight: 100.16

Accurate Mass: 100.088815

Percentage Composition: C 71.95%; H 12.08%; O 15.97%

Biological Source: Occurs in geranium, tea, citrus and other oils, and many fruits, e.g. banana, concord grape, quince

Use/Importance: Used as tea flavourant. Preferred to (*E*)-isomer in perfumes and flavours to add natural 'green' notes

Physical Description: Liq. with odour of fresh grass

Boiling Point: Bp 156-157°. Bp₁₉ 65-67°. Bp₂₀ 73.5-74.3°

Refractive Index: n_D^{20} 1.4384

Hazard & Toxicity: Flammable, fl. p. 54°, low oral tox.

Aldrich: W25630-7

Fluka: 53056

Sigma: H1265

>>Derivative: *O*-β-D-Glucopyranoside

Synonym(s): (*Z*)-3-Hexenyl β-D-glucopyranoside

CAS Registry Number: 95632-87-4

Molecular Formula: $\text{C}_{12}\text{H}_{22}\text{O}_6$

Molecular Weight: 262.302

Accurate Mass: 262.14164

Percentage Composition: C 54.95%; H 8.45%; O 36.60%

Biological Source: Isol. from leaves of *Pertya glabrescens* and from Danyshen (prob. *Codonopsis pilosula*)

Physical Description: Syrup

Melting Point: Mp 63° (as tetra-Ac)

Optical Rotation: $[\alpha]_D^{21}$ -38 (c, 0.48 in MeOH)