



>>Entry Name: 2-Hexen-1-ol, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2-Hexenyl alcohol. FEMA 2562

CAS Registry Number: 2305-21-7

Related CAS Registry Numbers(s): 2497-18-9 10094-40-3

$\text{H}_3\text{C}(\text{CH}_2)_2\text{CH}=\text{CHCH}_2\text{OH}$

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: 928-95-0

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: Isol. from tea. Constit. of many fruits, e.g., apples, grapes, and leaves. Defence chemical isol. from *Hotea gambiae*

Use/Importance: The alcohol and its simple esters, esp. the acetate, are used in perfumes and flavourings

Boiling Point: Bp 158-160°. Bp₉₅ 100.5-103.4°. Bp₂₀ 71.5-72°

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 3500 mg/kg

Aldrich: 13266-7

Fluka: 53057

>>Derivative: O-β-D-Glucopyranoside

Synonym(s): Erigeside B

CAS Registry Number: 117017-90-0

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 Chinese drug Dangshen (prob. *Codonopsis pilosula*). Also from *Erigeron breviscapus*

Physical Description: Syrup

Optical Rotation: $[\alpha]_{\text{D}}^{21} -28.3$ (c, 0.43 in EtOH)

>>Derivative: O-[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside]

CAS Registry Number: 129277-35-6

Molecular Formula: $\text{C}_{17}\text{H}_{30}\text{O}_{10}$

Molecular Weight: 394.418

Accurate Mass: 394.1839

Percentage Composition: C 51.77%; H 7.67%; O 40.56%

Biological Source: Constit. of *Codonopsis tangshen*

Physical Description: Syrup

Optical Rotation: $[\alpha]_{\text{D}}^{23} -26.7$ (c, 0.1 in H₂O)

>>Derivative: O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]

Synonym(s): 2-Hexenyl sophoroside

CAS Registry Number: 129277-34-5

Molecular Formula: $\text{C}_{18}\text{H}_{32}\text{O}_{11}$

Molecular Weight: 424.444

Accurate Mass: 424.194465

Percentage Composition: C 50.94%; H 7.60%; O 41.46%

Biological Source: Constit. of *Codonopsis tangshen*

Physical Description: Powder

Optical Rotation: $[\alpha]_{\text{D}}^{24} -25.7$ (c, 0.3 in H₂O)