



>>Entry Name: 1-Hexanol, 9CI

ENTRY UNDER REVIEW

Synonym(s): Hexyl alcohol, 8CI. Alcohol C6. Caproyl alcohol. FEMA 2567

CAS Registry Number: 111-27-3

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

$\text{H}_3\text{C}(\text{CH}_2)_4\text{CH}_2\text{OH}$

Molecular Formula: $\text{C}_6\text{H}_{14}\text{O}$

Molecular Weight: 102.176

Accurate Mass: 102.104465

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

Source/Synthesis: Common constit. of essential oils e.g. orange peel oil. Flavouring ingredient

Use/Importance: Used in perfumery

Physical Description: Oil with fruity/aromatic odour and flavour

Melting Point: Fp -46.7°

Boiling Point: Bp 157°

Density: d_{20}^{20} 0.8204

Refractive Index: n_D^{20} 1.4133

Hazard & Toxicity: Fl. p. 63° . Skin and eye irritant. LD₅₀ (rat, orl) 720 mg/kg

Aldrich: H1330-3

Fluka: 52840

Sigma: H4504

Supelco: R60-0235

>>Derivative: O- β -D-Glucopyranoside

Synonym(s): Hexyl glucoside

CAS Registry Number: 59080-45-4

Molecular Formula: $\text{C}_{12}\text{H}_{24}\text{O}_6$

Molecular Weight: 264.318

Accurate Mass: 264.15729

Percentage Composition: C 54.53%; H 9.15%; O 36.32%

Biological Source: Constit. of *Citrus* spp., *Codonopsis pilosula*, *Rhodiola quadrifida* and apples (*Malus sylvestris*)

Melting Point: Mp 51.5° (as tetra-Ac)

Optical Rotation: $[\alpha]_D -24.6$ (CHCl_3) (tetra-Ac)

>>Derivative: O-[β -D-Xylopyranosyl-(1 $\rightarrow$ 6)- β -D-glucopyranoside]

Molecular Formula: $\text{C}_{17}\text{H}_{32}\text{O}_{10}$

Molecular Weight: 396.434

Accurate Mass: 396.19955

Percentage Composition: C 51.51%; H 8.14%; O 40.36%

Biological Source: Constit. of *Rehmannia glutinosa*

Physical Description: Powder

Optical Rotation: $[\alpha]_D^{28} -48$ (c, 0.1 in MeOH)

>>Derivative: O-[β -D-Glucopyranosyl-(1 $\rightarrow$ 2)- β -D-glucopyranoside]

Synonym(s): Hexyl β -sophoroside

CAS Registry Number: 129277-37-8

Molecular Formula: $\text{C}_{18}\text{H}_{34}\text{O}_{11}$

Molecular Weight: 426.46

Accurate Mass: 426.210115

Percentage Composition: C 50.70%; H 8.04%; O 41.27%

Biological Source: Constit. of *Codonopsis tangshen*

Physical Description: Needles (MeOH)

Melting Point: Mp $198-199^\circ$

Optical Rotation: $[\alpha]_D^{24} -30.4$ (c, 1.4 in H_2O)