



>>Entry Name: 2,6-Dimethyl-4-heptanol, 9CI

ENTRY UNDER REVIEW

Synonym(s): Diisobutylcarbinol. FEMA 3140

CAS Registry Number: 108-82-7

Type of Compound Code(s): WE9999

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

Molecular Formula: $\text{C}_9\text{H}_{20}\text{O}$

Molecular Weight: 144.256

Accurate Mass: 144.151415

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

Boiling Point: Bp 179°. Bp₁₄ 72°

Solubility: Insol. H_2O , sol. EtOH, Et_2O

Density: d^{20}_4 0.81

Refractive Index: n^{20}_D 1.4238

Hazard & Toxicity: Eye, skin and respiratory tract irritant. Adverse hepatic and CNS effects reported by ingestion. LD₅₀ (rat, orl) 3160 mg/kg. LD₅₀ (rbt, skn) 4600 mg/kg

Aldrich: W31400-5

Rare Chemicals Library: S35073-7

>>Derivative: 1-Naphthylurethane

Melting Point: Mp 71-74°

>>Derivative: Ac

Molecular Formula: $\text{C}_{11}\text{H}_{22}\text{O}_2$

Molecular Weight: 186.294

Accurate Mass: 186.16198

Percentage Composition: C 70.92%; H 11.90%; O 17.18%

Boiling Point: Bp₆₀ 125-126°

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 188A, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 180A, (*ir*)

Ipatieff, V.N. *et al.*, *J.O.C.*, 1942, **7**, 189-198, (*synth*)

Sarel, S. *et al.*, *J.A.C.S.*, 1956, **78**, 5416-5420, (*Ac*)

Sokolova, E.B. *et al.*, *CA*, 1962, **56**, 8652, (*synth*)

Brown, H.C. *et al.*, *Synthesis*, 1978, 676-677, (*synth*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 178

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 856-857

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DNH800