



>>Entry Name: 6-Methyl-1-heptanol, 9CI

Synonym(s): Isooctanol

CAS Registry Number: 1653-40-3

Extra CAS Registry Numbers(s): 26952-21-6

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

Molecular Formula: $\text{C}_8\text{H}_{18}\text{O}$

Molecular Weight: 130.23

Accurate Mass: 130.135765

Percentage Composition: C 73.78%; H 13.93%; O 12.29%

Physical Description: Liq.

Boiling Point: Bp 187.6°. Bp₁₄ 87-89°

Rare Chemicals Library: S52134-5

>>Derivative: O-Sulfate

Molecular Formula: $\text{C}_8\text{H}_{18}\text{O}_4\text{S}$

Molecular Weight: 210.294

Accurate Mass: 210.09258

Percentage Composition: C 45.69%; H 8.63%; O 30.43%; S 15.25%

Biological Source: Isol. from the ascidian *Halocynthia papillosa*

Physical Description: Amorph. solid

>>Derivative: Phenylurethane

Melting Point: Mp 81-81.4°

References:

Levene, P.A. *et al.*, *J. Biol. Chem.*, 1916, **27**, 452

Dorough, G.L. *et al.*, *J.A.C.S.*, 1941, **63**, 3100-3110, (*synth*)

Bestmann, H.J. *et al.*, *Chem. Ber.*, 1976, **109**, 3375-3378, (*synth*)

Aiello, A. *et al.*, *J. Nat. Prod.*, 2000, **63**, 1590-1592, (*isol, sulfate*)