



>>Entry Name: 4-Heptanol, 9CI

CAS Registry Number: 589-55-9

Extra CAS Registry Numbers(s): 53535-33-4

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

Molecular Formula: $\text{C}_7\text{H}_{16}\text{O}$

Molecular Weight: 116.203

Accurate Mass: 116.120115

Percentage Composition: C 72.35%; H 13.88%; O 13.77%

Melting Point: Fp -41.5°

Boiling Point: Bp 154° . Bp₁₆ 63.8°

Hazard & Toxicity: Flammable, fl. p. 49°

Fluka: 51830

Rare Chemicals Library: S45512-1

>>Derivative: 3-Octadecenoyl(Z-)

Synonym(s): 1-Propylbutyl 3-octadecenoate

Molecular Formula: $\text{C}_{25}\text{H}_{48}\text{O}_2$

Molecular Weight: 380.653

Accurate Mass: 380.36543

Percentage Composition: C 78.88%; H 12.71%; O 8.41%

Biological Source: Constit. of the fruit of *Fagara budrunga*

Physical Description: Pale yellow liq.

UV: [neutral] λ_{max} 210 (ϵ 200) (MeOH)

>>Derivative: Benzoyl

Molecular Formula: $\text{C}_{14}\text{H}_{20}\text{O}_2$

Molecular Weight: 220.311

Accurate Mass: 220.14633

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Boiling Point: Bp₁₄ $146-147^\circ$

References:

Lund, H., *Ber.*, 1937, **70**, 1523, (*synth*)

Pearce, P.J., *J.C.S. Perkin I*, 1972, 1655, (*synth*)

Naik, D.G. *et al.*, *Indian J. Chem., Sect. B*, 1999, **38**, 122-124, (*3-octadecenoate*)