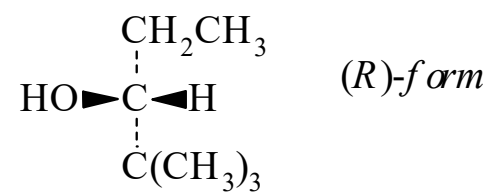




>>Entry Name: 2,2-Dimethyl-3-pentanol

Synonym(s): *tert*-Butylethylcarbinol



CAS Registry Number: 3970-62-5

Molecular Formula: C<sub>7</sub>H<sub>16</sub>O

Molecular Weight: 116.203

Accurate Mass: 116.120115

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

Aldrich: D17362-2

>>Variant: (*R*)-form

CAS Registry Number: 38636-36-1

Molecular Formula: C<sub>7</sub>H<sub>16</sub>O

Molecular Weight: 116.203

Accurate Mass: 116.120115

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

Physical Description: Liq.

Boiling Point: Bp 132-135°. Bp<sub>15</sub> 42-44°

Refractive Index: n<sub>D</sub><sup>20</sup> 1.4230

>>Derivative: Ac

Molecular Formula: C<sub>9</sub>H<sub>18</sub>O<sub>2</sub>

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Boiling Point: Bp<sub>38</sub> 74°

Optical Rotation: [α]<sub>D</sub><sup>24</sup> +12.16 (neat)

Density: d<sup>23</sup> 0.856

Refractive Index: n<sub>D</sub><sup>20</sup> 1.4103

>>Variant: (±)-form

Molecular Formula: C<sub>7</sub>H<sub>16</sub>O

Molecular Weight: 116.203

Accurate Mass: 116.120115

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

Physical Description: Liq. with camphoraceous odour

Boiling Point: Bp 132-135°

Density: d<sub>4</sub><sup>0</sup> 0.841

>>Derivative: Ac

CAS Registry Number: 39511-81-4

Physical Description: Liq.

Boiling Point: Bp<sub>770</sub> 157-159°

#### References:

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 186A, (*nmr*)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 124A, (*ir*)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 175A, (*ir*)

Favorskii, A., *J. Prakt. Chem.*, 1913, **88**, 675, (*synth*)

Whitmore, E.C. *et al.*, *J.A.C.S.*, 1942, **64**, 2966, (*synth*)

Cavalieri, L. *et al.*, *J.A.C.S.*, 1945, **67**, 1784, (*synth*)

Foley, W.M. *et al.*, *J.A.C.S.*, 1959, **81**, 2779, (*resoln, abs config*)

Battioni, J.P., *Bull. Soc. Chim. Fr.*, 1972, 2068