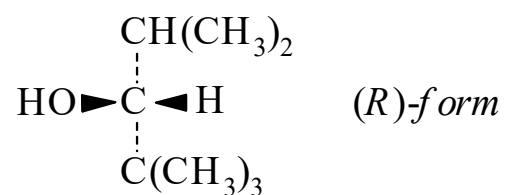




>>Entry Name: 2,2,4-Trimethyl-3-pentanol, 9CI, 8CI

Synonym(s): *tert*-Butylisopropylcarbinol



CAS Registry Number: 5162-48-1

Molecular Formula: C<sub>8</sub>H<sub>18</sub>O

Molecular Weight: 130.23

Accurate Mass: 130.135765

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

Rare Chemicals Library: S41197-3

>>Variant: (*R*)-form

CAS Registry Number: 63726-56-7

Molecular Formula: C<sub>8</sub>H<sub>18</sub>O

Molecular Weight: 130.23

Accurate Mass: 130.135765

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

Optical Rotation:  $[\alpha]_{\text{D}}^{28} +9.06$  (neat)

>>Variant: (*S*)-form

Molecular Formula: C<sub>8</sub>H<sub>18</sub>O

Molecular Weight: 130.23

Accurate Mass: 130.135765

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

Optical Rotation:  $[\alpha]_{\text{D}}^{28} -8.94$  (neat)

>>Variant: ( $\pm$ )-form

CAS Registry Number: 63783-31-3

Molecular Formula: C<sub>8</sub>H<sub>18</sub>O

Molecular Weight: 130.23

Accurate Mass: 130.135765

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

Physical Description: Liq.

Melting Point: Mp  $-13^{\circ}$

Boiling Point: Bp  $151^{\circ}$

Density:  $d_4^{20}$  0.83

>>Derivative: 3,5-Dinitrobenzoyl

Melting Point: Mp  $101\text{-}102^{\circ}$

>>Derivative: Phenylurethane

Molecular Formula: C<sub>15</sub>H<sub>23</sub>NO<sub>2</sub>

Molecular Weight: 249.352

Accurate Mass: 249.172879

Percentage Composition: C 72.25%; H 9.30%; N 5.62%; O 12.83%

Melting Point: Mp  $79^{\circ}$

#### References:

Whitmore, F.C. *et al.*, *J.A.C.S.*, 1932, **54**, 3714, (*synth*)

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