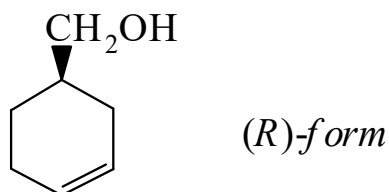




>>Entry Name: 3-Cyclohexene-1-methanol, 9CI

Synonym(s): 4-Hydroxymethylcyclohexene. 1,2,3,6-Tetrahydrobenzyl alcohol



CAS Registry Number: 1679-51-2

Molecular Formula: C<sub>7</sub>H<sub>12</sub>O

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Use/Importance: Biological precursor of 2-Methylene-3-oxocyclopentanecarboxylic acid [HDW48-R](#)

Aldrich: 16216-7

Fluka: 87329

>>Variant: (R)-form

CAS Registry Number: 5709-99-9

Molecular Formula: C<sub>7</sub>H<sub>12</sub>O

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Optical Rotation: [α]<sub>D</sub> +104 (c, 6 in CHCl<sub>3</sub>)

>>Derivative: 4-Methylbenzenesulfonyl

Melting Point: Mp 22-24°

>>Variant: (S)-form

CAS Registry Number: 5681-56-1

Molecular Formula: C<sub>7</sub>H<sub>12</sub>O

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Boiling Point: Bp<sub>0.6</sub> 62-63°

Optical Rotation: [α]<sub>D</sub><sup>24</sup> -105 (c, 3.5 in CH<sub>2</sub>Cl<sub>2</sub>)

>>Variant: (±)-form

CAS Registry Number: 72581-32-9

Molecular Formula: C<sub>7</sub>H<sub>12</sub>O

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Boiling Point: Bp<sub>10</sub> 90.5°

>>Derivative: Ac

CAS Registry Number: 20144-30-3

Molecular Formula: C<sub>9</sub>H<sub>14</sub>O<sub>2</sub>

Molecular Weight: 154.208

Accurate Mass: 154.09938

Percentage Composition: C 70.10%; H 9.15%; O 20.75%

Boiling Point: Bp<sub>10</sub> 78°

References: