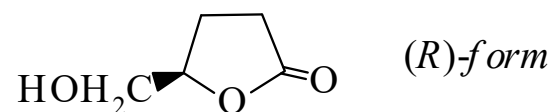




>>Entry Name: 4,5-Dihydro-5-(hydroxymethyl)-2(3*H*)-furanone, 9CI

Synonym(s): 4,5-Dihydroxypentanoic acid  $\gamma$ -lactone, 8CI.  $\gamma$ -Hydroxymethyl- $\gamma$ -butyrolactone. 5-Hydroxy-4-pentanolide



CAS Registry Number: 10374-51-3

Molecular Formula: C<sub>5</sub>H<sub>8</sub>O<sub>3</sub>

Molecular Weight: 116.116

Accurate Mass: 116.047345

Percentage Composition: C 51.72%; H 6.94%; O 41.34%

>>Variant: (*R*)-form

CAS Registry Number: 52813-63-5

Molecular Formula: C<sub>5</sub>H<sub>8</sub>O<sub>3</sub>

Molecular Weight: 116.116

Accurate Mass: 116.047345

Percentage Composition: C 51.72%; H 6.94%; O 41.34%

Physical Description: Liq.

Boiling Point: Bp<sub>0.048</sub> 101-102°

Optical Rotation:  $[\alpha]_D^{30}$  -33.5 (c, 3.12 in EtOH).  $[\alpha]_D^{20}$  -54.5 (c, 2.0 in CHCl<sub>3</sub>) (>96% ee)

Aldrich: 34354-4

Fluka: 55621

>>Derivative: *O*-Triphenylmethyl

CAS Registry Number: 78158-90-4

Molecular Formula: C<sub>24</sub>H<sub>22</sub>O<sub>3</sub>

Molecular Weight: 358.436

Accurate Mass: 358.156895

Percentage Composition: C 80.42%; H 6.19%; O 13.39%

Melting Point: Mp 152-154°

Optical Rotation:  $[\alpha]_D^{20}$  -26.5 (c, 1 in CHCl<sub>3</sub>)

Aldrich: 43897-9

Fluka: 93461

Other: Kiralchem

>>Variant: (*S*)-form

CAS Registry Number: 32780-06-6

Molecular Formula: C<sub>5</sub>H<sub>8</sub>O<sub>3</sub>

Molecular Weight: 116.116

Accurate Mass: 116.047345

Percentage Composition: C 51.72%; H 6.94%; O 41.34%

Physical Description: Liq.

Boiling Point: Bp<sub>7</sub> 131-147°

Optical Rotation:  $[\alpha]_D^{26}$  +31.3 (c, 2.92 in EtOH)

Aldrich: 34890-2

Fluka: 55620

>>Derivative: Benzoyl

CAS Registry Number: 32780-07-7

Molecular Formula: C<sub>12</sub>H<sub>12</sub>O<sub>4</sub>

Molecular Weight: 220.224

Accurate Mass: 220.07356

Percentage Composition: C 65.45%; H 5.49%; O 29.06%

Physical Description: Needles (C<sub>6</sub>H<sub>6</sub>/hexane)

Melting Point: Mp 59-60.5°

Optical Rotation:  $[\alpha]_D^{26}$  +48.2 (c, 1.03 in EtOH)

>>Derivative: 4-Methylbenzenesulfonyl

CAS Registry Number: 58879-34-8

Melting Point: Mp 86-88°