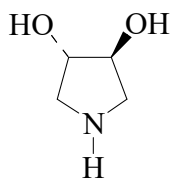




>>Entry Name: 3,4-Pyrrolidinediol, 9Cl



(3*S*,4*S*)-form

Related CAS Registry Numbers(s): 136779-52-7

Molecular Formula: C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>

Molecular Weight: 103.121

Accurate Mass: 103.063329

Percentage Composition: C 46.59%; H 8.80%; N 13.58%; O 31.03%

>>Variant: (3*S*,4*S*)-form

Synonym(s): (+)-*trans*-form

CAS Registry Number: 90481-32-6

Molecular Formula: C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>

Molecular Weight: 103.121

Accurate Mass: 103.063329

Percentage Composition: C 46.59%; H 8.80%; N 13.58%; O 31.03%

Physical Description: Cryst. by subl.

Melting Point: Mp 101-103°

Optical Rotation:  $[\alpha]_{\text{D}}^{25} +24.9$  (c, 2.13 in EtOH)

Other Data: Racemate known but not well characterised

>>Derivative: *N*-Benzyl

CAS Registry Number: 90365-74-5

Molecular Formula: C<sub>11</sub>H<sub>15</sub>NO<sub>2</sub>

Molecular Weight: 193.245

Accurate Mass: 193.110279

Percentage Composition: C 68.37%; H 7.82%; N 7.25%; O 16.56%

Physical Description: Cryst. solid (Et<sub>2</sub>O)

Melting Point: Mp 100°

Optical Rotation:  $[\alpha]_{\text{D}}^{20} +31.4$  (c, 4 in MeOH)

>>Derivative: *N-tert*-Butyloxycarbonyl

CAS Registry Number: 90481-33-7

Molecular Formula: C<sub>9</sub>H<sub>17</sub>NO<sub>4</sub>

Molecular Weight: 203.238

Accurate Mass: 203.115759

Percentage Composition: C 53.19%; H 8.43%; N 6.89%; O 31.49%

Physical Description: Cryst. (toluene/AcOH)

Melting Point: Mp 163-165°

Optical Rotation:  $[\alpha]_{\text{D}}^{25} -21.9$  (c, 3.065 in MeOH)

>>Derivative: Bis(methoxymethyl) ether

CAS Registry Number: 138051-80-6

Molecular Formula: C<sub>8</sub>H<sub>17</sub>NO<sub>4</sub>

Molecular Weight: 191.227

Accurate Mass: 191.115759

Percentage Composition: C 50.25%; H 8.96%; N 7.32%; O 33.47%

Physical Description: Pale yellow oil

Optical Rotation:  $[\alpha]_{\text{D}}^{20} -1.51$  (c, 6.4 in CHCl<sub>3</sub>)

>>Derivative: Bis(methoxymethyl) ether, *N*-benzyl

CAS Registry Number: 137945-72-3

Molecular Formula: C<sub>15</sub>H<sub>23</sub>NO<sub>4</sub>

Molecular Weight: 281.351

Accurate Mass: 281.162709

Percentage Composition: C 64.04%; H 8.24%; N 4.98%; O 22.75%

Physical Description: Oil

Optical Rotation:  $[\alpha]_{\text{D}}^{20} +11.9$  (c, 2.4 in CHCl<sub>3</sub>)