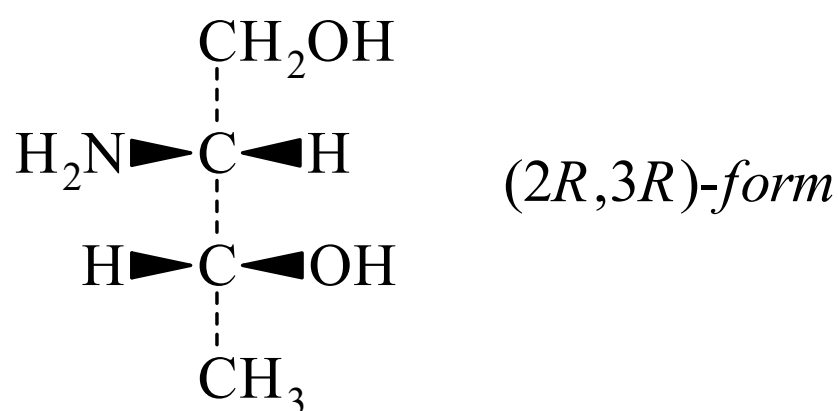




>>Entry Name: 2-Amino-1,3-butanediol, 9CI



CAS Registry Number: 31066-40-7

Related CAS Registry Numbers(s): 515-93-5 4493-96-3

Molecular Formula: C<sub>4</sub>H<sub>11</sub>NO<sub>2</sub>

Molecular Weight: 105.136

Accurate Mass: 105.078979

Percentage Composition: C 45.70%; H 10.55%; N 13.32%; O 30.44%

>>Variant: (2*R*,3*R*)-form

Synonym(s): L-Threoninol

CAS Registry Number: 3228-51-1

Molecular Formula: C<sub>4</sub>H<sub>11</sub>NO<sub>2</sub>

Molecular Weight: 105.136

Accurate Mass: 105.078979

Percentage Composition: C 45.70%; H 10.55%; N 13.32%; O 30.44%

Aldrich: 46996-3

Other: Degussa

>>Derivative: Oxalate (1:1)

Molecular Formula: C<sub>6</sub>H<sub>13</sub>NO<sub>6</sub>

Molecular Weight: 195.172

Percentage Composition: C 36.92%; H 6.71%; N 7.18%; O 49.19%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 188.5-189°

Optical Rotation:  $[\alpha]_{\text{D}}^{25} -7.84$  (c, 0.9 in H<sub>2</sub>O)

>>Variant: (2*R*,3*S*)-form

Synonym(s): L-Allothreoninol

CAS Registry Number: 108102-48-3

Molecular Formula: C<sub>4</sub>H<sub>11</sub>NO<sub>2</sub>

Molecular Weight: 105.136

Accurate Mass: 105.078979

Percentage Composition: C 45.70%; H 10.55%; N 13.32%; O 30.44%

>>Derivative: Oxalate (1:1)

Molecular Formula: C<sub>6</sub>H<sub>13</sub>NO<sub>6</sub>

Molecular Weight: 195.172

Percentage Composition: C 36.92%; H 6.71%; N 7.18%; O 49.19%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 175-176°

Optical Rotation:  $[\alpha]_{\text{D}}^{25} -27.26$  (c, 0.73 in H<sub>2</sub>O)

>>Variant: (2*S*,3*R*)-form

Synonym(s): D-Allothreoninol

CAS Registry Number: 44520-54-9

Molecular Formula: C<sub>4</sub>H<sub>11</sub>NO<sub>2</sub>

Molecular Weight: 105.136

Accurate Mass: 105.078979

Percentage Composition: C 45.70%; H 10.55%; N 13.32%; O 30.44%