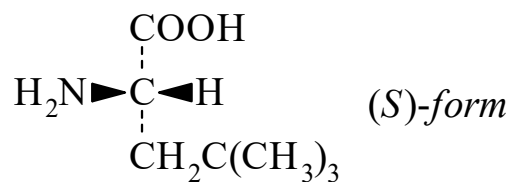




>>Entry Name: 2-Amino-4,4-dimethylpentanoic acid

Synonym(s): 4-Methylleucine, 9Cl. Neopentylglycine



Molecular Formula: C<sub>7</sub>H<sub>15</sub>NO<sub>2</sub>

Molecular Weight: 145.201

Accurate Mass: 145.110279

Percentage Composition: C 57.90%; H 10.41%; N 9.65%; O 22.04%

>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 57224-50-7

Molecular Formula: C<sub>7</sub>H<sub>15</sub>NO<sub>2</sub>

Molecular Weight: 145.201

Accurate Mass: 145.110279

Percentage Composition: C 57.90%; H 10.41%; N 9.65%; O 22.04%

Melting Point: Mp 259-260°

Optical Rotation: [α]<sub>D</sub> +14.7 (AcOH)

Other Data: (R)-form also known

Sigma: M3893

>>Derivative: N-tert-Butyloxycarbonyl

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

Melting Point: Mp 102-103°

Optical Rotation: [α]<sub>D</sub> +14 (MeOH)

>>Derivative: N-Formyl

Molecular Formula: C<sub>8</sub>H<sub>15</sub>NO<sub>3</sub>

Molecular Weight: 173.211

Accurate Mass: 173.105194

Percentage Composition: C 55.47%; H 8.73%; N 8.09%; O 27.71%

Melting Point: Mp 175-177°

Optical Rotation: [α]<sub>D</sub> -13 (EtOH)

>>Derivative: N-Ac

Molecular Formula: C<sub>9</sub>H<sub>17</sub>NO<sub>3</sub>

Molecular Weight: 187.238

Accurate Mass: 187.120844

Percentage Composition: C 57.73%; H 9.15%; N 7.48%; O 25.63%

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

Melting Point: Mp 224-225°

>>Variant: (±)-form

CAS Registry Number: 60122-72-7

Molecular Formula: C<sub>7</sub>H<sub>15</sub>NO<sub>2</sub>

Molecular Weight: 145.201

Accurate Mass: 145.110279

Percentage Composition: C 57.90%; H 10.41%; N 9.65%; O 22.04%

Melting Point: Mp 235-237 dec.°

Fluka: 72138

Sigma: M4018

>>Derivative: N-Formyl

Physical Description: Cryst. (EtOH/C<sub>6</sub>H<sub>6</sub>)

Melting Point: Mp 162-163°

References: