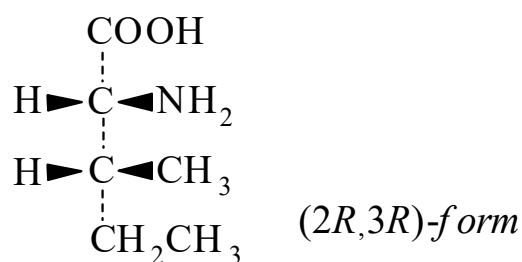




>>Entry Name: 2-Amino-3-methylpentanoic acid

ENTRY UNDER REVIEW

Synonym(s): 3-Methylnorvaline. Isoleucine. Ile



CAS Registry Number: 7004-09-3

Related CAS Registry Numbers(s): 4125-98-8 10466-56-5 18598-74-8

Molecular Formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>

Molecular Weight: 131.174

Accurate Mass: 131.094629

Percentage Composition: C 54.94%; H 9.99%; N 10.68%; O 24.39%

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

Synonym(s): D-erythro-form. D-Isoleucine

CAS Registry Number: 319-78-8

Molecular Formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>

Molecular Weight: 131.174

Accurate Mass: 131.094629

Percentage Composition: C 54.94%; H 9.99%; N 10.68%; O 24.39%

Biological Source: From numerous peptide antibiotics

Melting Point: Mp 283-284 dec.°

Optical Rotation:  $[\alpha]_{\text{D}}^{20} -12.2$  (c, 3.2 in H<sub>2</sub>O).  $[\alpha]_{\text{D}} -41$  (c, 1 in 5M HCl)

Aldrich: 29865-4

Sigma: I7634

>>Derivative: Me ester; hydrochloride

Melting Point: Mp 98-100°

Optical Rotation:  $[\alpha]_{\text{D}}^{20} -26.6$  (c, 2 in H<sub>2</sub>O)

>>Derivative: Et ester

CAS Registry Number: 3082-86-8

Molecular Formula: C<sub>8</sub>H<sub>17</sub>NO<sub>2</sub>

Molecular Weight: 159.228

Accurate Mass: 159.125929

Percentage Composition: C 60.35%; H 10.76%; N 8.80%; O 20.10%

Physical Description: Oil

>>Derivative: Amide; hydrochloride

CAS Registry Number: 104602-68-8

Melting Point: Mp 247-248°

Optical Rotation:  $[\alpha]_{\text{D}}^{20} -21$  (c, 1 in H<sub>2</sub>O)

>>Derivative: N-Formyl

Melting Point: Mp 156°

Optical Rotation:  $[\alpha]_{\text{D}}^{25} -26.8$  (EtOH)

>>Derivative: N-Ac

CAS Registry Number: 19764-31-9

Physical Description: Cryst. (H<sub>2</sub>O or Me<sub>2</sub>CO)

Melting Point: Mp 150-151°

Optical Rotation:  $[\alpha]_{\text{D}}^{25} -15$  (c, 2 in EtOH).  $[\alpha]_{\text{D}} +25.2$  (c, 2 in Me<sub>2</sub>CO).  $[\alpha]_{\text{D}} +82.6$  (c, 2 in H<sub>2</sub>O)