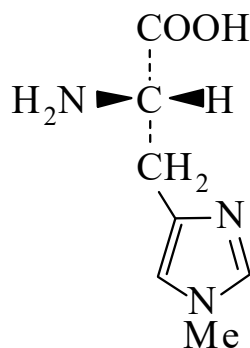




>>Entry Name: 1-Methylhistidine, 9Cl

ENTRY UNDER REVIEW

Synonym(s): 2-Amino-3-(1-methyl-4-imidazolyl)propanoic acid. N^T -Methylhistidine. **3-Methylhistidine**‡



Molecular Formula: C₇H₁₁N₃O₂

Molecular Weight: 169.183

Accurate Mass: 169.085127

Percentage Composition: C 49.70%; H 6.55%; N 24.84%; O 18.91%

Metabolism: Protein metabolite

Other Data: Frequently referred to as 3-methylhistidine in biochemical papers due to the long-standing difference in the numbering of histidine

>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 332-80-9

Molecular Formula: C₇H₁₁N₃O₂

Molecular Weight: 169.183

Accurate Mass: 169.085127

Percentage Composition: C 49.70%; H 6.55%; N 24.84%; O 18.91%

Biological Source: Nonproteinogenic amino acid formed mainly by methylation of histidine residues in muscle actin and myosin. Urinary excretion levels used as an index of muscle protein breakdown

Physical Description: Plates (DMF aq.)

Melting Point: Mp 248-250 dec.°

Optical Rotation: $[\alpha]_D^{20}$ -24.7 (c, 2.8 in H₂O)

pKa Value: pK_{a2} 6.56; pK_{a3} 8.73 (25°, 0.1M KCl)

Sigma: M9005

>>Derivative: Hydrochloride

Physical Description: Plates (DMF aq.)

Melting Point: Mp 251-252 dec.°

Optical Rotation: $[\alpha]_D^{22}$ +6.9 (c, 2.0 in H₂O). $[\alpha]_D$ +9.4 (c, 2.0 in M HCl)

>>Derivative: Hydrochloride (1:2)

CAS Registry Number: 69614-06-8

Physical Description: Prisms

Melting Point: Mp 258-259°

Optical Rotation: $[\alpha]_D^{20}$ +12.9 (c, 2 in M HCl)

References:

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Dunnett, M. *et al.*, *J. Chromatogr., B: Biomed. Appl.*, 1997, **688**, 47-55, (*hplc*)

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