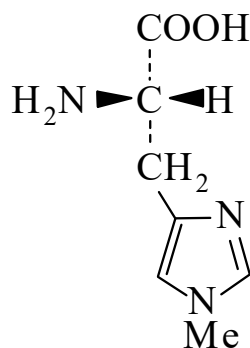




>>Entry Name: 1-Methylhistidine, 9Cl

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:

- Greenstein, J.P. *et al.*, *Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 2763, (*synth*)
Cocks, D.H. *et al.*, *Nature (London)*, 1964, **202**, 184, (*isol*)
Anon, *Eur. J. Biochem.*, 1972, **27**, 201-207, (*nomencl*)
Barlos, K. *et al.*, *Annalen*, 1989, 387, (*synth*)
Betto, P. *et al.*, *J. Chromatogr.*, 1992, **584**, 256-260, (*detm, hplc, use, bibl*)
Jain, R. *et al.*, *Tetrahedron*, 1996, **52**, 5363-5370, (*synth, pmr*)
Dunnett, M. *et al.*, *J. Chromatogr., B: Biomed. Appl.*, 1997, **688**, 47-55, (*hplc*)
Dunnett, M. *et al.*, *J. Chromatogr., B: Biomed. Appl.*, 1997, **688**, 47-55, (*hplc*)
Garlick, P.J. *et al.*, *J. Nutr.*, Suppl. 2, 1998, **128**, 3565-3595, (*rev*)
Garlick, P.J. *et al.*, *J. Nutr.*, 2 Suppl., 1998, **128**, 3565-3595, (*rev*)
Colombani, P.C. *et al.*, *Int. J. Sport Nutr.*, 1999, **9**, 181-201, (*biochem*)
Colombani, P.C. *et al.*, *Int. J. Sport Nutr.*, 1999, **9**, 181-201, (*biochem*)