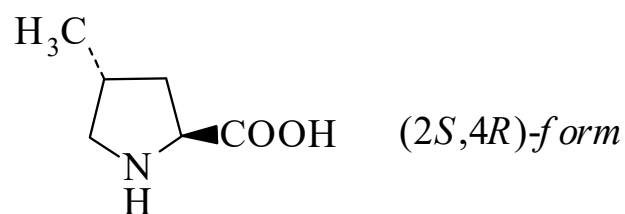




>>Entry Name: 4-Methyl-2-pyrrolidinecarboxylic acid

ENTRY UNDER REVIEW

Synonym(s): 4-Methylproline, 9Cl



Molecular Formula: C₆H₁₁NO₂

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

>>Variant: (2R,4R)-form

Synonym(s): D-*cis*-form

CAS Registry Number: 31137-95-8

Molecular Formula: C₆H₁₁NO₂

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

Melting Point: Mp 238-239 dec.°

Optical Rotation: $[\alpha]_D^{20} +85.2$ (c, 1.68 in H₂O). $[\alpha]_D +47.9$ (c, 1.28 in 3M HCl)

>>Variant: (2S,4R)-form

Synonym(s): L-*trans*-form

CAS Registry Number: 23009-50-9

Molecular Formula: C₆H₁₁NO₂

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

Biological Source: Constit. of young apple fruit and perry

Physical Description: Needles (EtOH/Et₂O)

Melting Point: Mp 239-240 dec.°

Optical Rotation: $[\alpha]_D^{18} -56.6$ (c, 1.03 in H₂O). $[\alpha]_D^{20} -23.9$ (c, 1.54 in 3M HCl)

>>Variant: (2S,4S)-form

Synonym(s): L-*cis*-form

CAS Registry Number: 6734-41-4

Molecular Formula: C₆H₁₁NO₂

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

Biological Source: Present in hydrolysate of antibiotic ICI 13959

Physical Description: Cryst. (EtOH/Et₂O)

Optical Rotation: $[\alpha]_D^{18} -83$ (c, 0.53 in H₂O). $[\alpha]_D -43$ (c, 0.51 in 3M HCl)

References:

Dalby, J.S. *et al.*, *J.C.S.*, 1962, 4387, (*synth*)

Wang, Q. *et al.*, *Tetrahedron*, 1998, **54**, 15759-15780, (*2S,4R-form, synth, ir, pmr, cmr*)