



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

Synonym(s): 2-Methylproline, 9CI



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: (R)-form

CAS Registry Number: 63399-77-9

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%

Physical Description: Ppt. (MeOH/Et₂O)

Melting Point: Mp 330 dec.°

Optical Rotation: [α]_D²⁰ +75.3 (c, 1 in MeOH)

>>Variant: (S)-form

CAS Registry Number: 42856-71-3

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 248-252°

Optical Rotation: [α]_D²⁵ -71.2 (c, 1.0 in MeOH)

>>Derivative: Me ester

CAS Registry Number: 109837-32-3

Molecular Formula: C₇H₁₃NO₂

Molecular Weight: 143.185

Accurate Mass: 143.094629

Percentage Composition: C 58.72%; H 9.15%; N 9.78%; O 22.35%

Physical Description: Cryst. (MeOH/EtOAc) (as hydrochloride)

Melting Point: Mp 106-108° (hydrochloride)

>>Derivative: *N*-tert-Butyloxycarbonyl

Molecular Formula: C₁₁H₁₉NO₄

Molecular Weight: 229.275

Accurate Mass: 229.131409

Percentage Composition: C 57.63%; H 8.35%; N 6.11%; O 27.91%

Physical Description: Pale yellow cryst.

Melting Point: Mp 129-130°

Optical Rotation: [α]_D -50.6 (c, 1.4 in CHCl₃)

>>Variant: (±)-form

CAS Registry Number: 16277-06-8

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%

Physical Description: Cryst. (MeOH/Et₂O)

Melting Point: Mp 263-264.5°

References: