



>>Entry Name: Proline, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2-Pyrrolidinecarboxylic acid. Tetrahydro-2-pyrrolecarboxylic acid. Pro



CAS Registry Number: 7005-20-1

Related CAS Registry Numbers(s): 16395-58-7

Molecular Formula: C₅H₉NO₂

Molecular Weight: 115.132

Accurate Mass: 115.063329

Percentage Composition: C 52.16%; H 7.88%; N 12.17%; O 27.79%

>>Variant: (*R*)-form

Synonym(s): D-form

CAS Registry Number: 344-25-2

Molecular Formula: C₅H₉NO₂

Molecular Weight: 115.132

Accurate Mass: 115.063329

Percentage Composition: C 52.16%; H 7.88%; N 12.17%; O 27.79%

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 206° (215-220° dec.)

Optical Rotation: $[\alpha]_D^{20} +86.2$ (c, 1.0 in H₂O) (100% op). $[\alpha]_D +60.4$ (c, 1 in 5M HCl)

Aldrich: 85891-9

Fluka: 81705

Sigma: P4266

>>Derivative: Me ester

CAS Registry Number: 43041-12-9

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: Oil

Optical Rotation: $[\alpha]_D^{25} +34$

>>Derivative: Et ester

CAS Registry Number: 96163-72-3

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: Oil

Optical Rotation: $[\alpha]_D^{20} +85.6$ (c, 2 in H₂O)

>>Derivative: Amide

Synonym(s): 2-Pyrrolidinecarboxamide, 9CI. Prolinamide

CAS Registry Number: 62937-45-5

Molecular Formula: C₅H₁₀N₂O

Molecular Weight: 114.147

Accurate Mass: 114.079313

Percentage Composition: C 52.61%; H 8.83%; N 24.54%; O 14.02%

Physical Description: Cryst.

Melting Point: Mp 97-98°

>>Derivative: *N*-tert-Butyloxycarbonyl