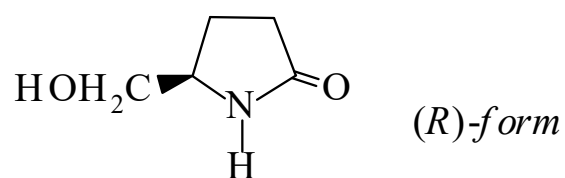




>>Entry Name: 5-(Hydroxymethyl)-2-pyrrolidinone, 9CI

Synonym(s): Pyroglutaminol



CAS Registry Number: 62400-75-3

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

CAS Registry Number: 66673-40-3

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. (EtOAc/CHCl₃)

Melting Point: Mp 73-74° (61-63°)

Optical Rotation: [α]_D²⁶ -33.3 (c, 1.76 in EtOH)

Fluka: 55820

>>Derivative: O-Triphenylmethyl

Molecular Formula: C₂₄H₂₃NO₂

Molecular Weight: 357.451

Accurate Mass: 357.172879

Percentage Composition: C 80.64%; H 6.49%; N 3.92%; O 8.95%

Melting Point: Mp 165-167°

Optical Rotation: [α]_D²⁰ -15.8 (c, 2 in CHCl₃)

Other: Kiralchem

>>Variant: (S)-form

CAS Registry Number: 17342-08-4

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.

Melting Point: Mp 86-87° (65-68°)

Boiling Point: Bp_{0.04} 148°

Optical Rotation: [α]_D²⁰ +34.5 (c, 1.04 in EtOH)

Aldrich: 36636-6

Fluka: 55830

>>Derivative: O-(4-Methylbenzenesulfonyl)

CAS Registry Number: 51693-17-5

Physical Description: Solid (toluene)

Melting Point: Mp 129-130°

Aldrich: 44453-7

>>Derivative: O-Triphenylmethyl

CAS Registry Number: 105526-85-0

Molecular Formula: C₂₄H₂₃NO₂

Molecular Weight: 357.451

Accurate Mass: 357.172879

Percentage Composition: C 80.64%; H 6.49%; N 3.92%; O 8.95%

Use/Importance: Used in asym. Diels-Alder reactions and asym. conjugate addns.

Melting Point: Mp 164-166°