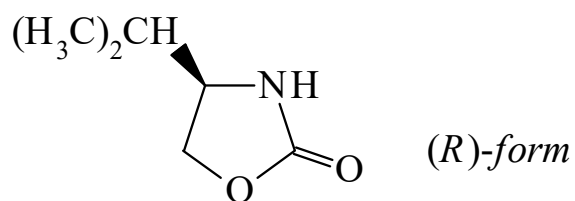




>>Entry Name: 4-Isopropyl-2-oxazolidinone

Synonym(s): 4-(1-Methylethyl)-2-oxazolidinone, 9CI



CAS Registry Number: 103723-70-2

Related CAS Registry Numbers(s): 96021-69-1 102922-29-2

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%

Use/Importance: Derivs. used as chiral auxiliaries in synth.

>>Variant: (R)-form

CAS Registry Number: 95530-58-8

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. (Et₂O)

Melting Point: Mp 70-72°

Optical Rotation: [α]_D −15.5 (c, 0.0706 in CHCl₃)

Aldrich: 33994-6

Fluka: 59658

>>Derivative: N-Propanoyl

CAS Registry Number: 89028-40-0

Molecular Formula: C₉H₁₅NO₃

Molecular Weight: 185.222

Accurate Mass: 185.105194

Percentage Composition: C 58.36%; H 8.16%; N 7.56%; O 25.91%

Use/Importance: Chiral auxiliary

Optical Rotation: [α]_D²⁰ −90 (c, 8.5 in CHCl₃)

>>Derivative: N-(2E-Butenoyl)

CAS Registry Number: 147511-27-1

Molecular Formula: C₁₀H₁₅NO₃

Molecular Weight: 197.233

Accurate Mass: 197.105194

Percentage Composition: C 60.90%; H 7.67%; N 7.10%; O 24.34%

Use/Importance: Chiral auxiliary

Melting Point: Mp 56°

Optical Rotation: [α]_D²⁵ −105 (c, 2 in CHCl₃)

>>Derivative: N-Phenylacetyl

CAS Registry Number: 103422-95-3

Molecular Formula: C₁₄H₁₇NO₃

Molecular Weight: 247.293

Accurate Mass: 247.120844

Percentage Composition: C 68.00%; H 6.93%; N 5.66%; O 19.41%

Use/Importance: Chiral auxiliary

Optical Rotation: [α]_D −82.9 (c, 2.6 in CHCl₃)

>>Variant: (S)-form