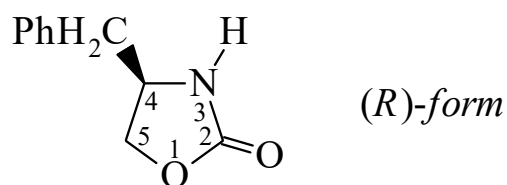




>>Entry Name: 4-Benzyl-2-oxazolidinone, 8Cl
Synonym(s): 4-(Phenylmethyl)-2-oxazolidinone, 9Cl



CAS Registry Number: 40217-17-2

Molecular Formula: C₁₀H₁₁NO₂

Molecular Weight: 177.202

Accurate Mass: 177.078979

Percentage Composition: C 67.78%; H 6.26%; N 7.90%; O 18.06%

Use/Importance: *N*-Acyl derivs. are used industrially in chiral synth. of amino acids and β-lactam antibiotics

>>Variant: (R)-form

CAS Registry Number: 102029-44-7

Molecular Formula: C₁₀H₁₁NO₂

Molecular Weight: 177.202

Accurate Mass: 177.078979

Percentage Composition: C 67.78%; H 6.26%; N 7.90%; O 18.06%

Use/Importance: Chiral reagent and auxiliary

Biological Use/Importance: Penetration enhancer for topical pharmaceuticals

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 88-90°

Optical Rotation: [α]_D²⁵+64 (c, 1 in CHCl₃)

Aldrich: 30097-7

Fluka: 13615

Sigma: B7268

>>Variant: (S)-form

CAS Registry Number: 90719-32-7

Molecular Formula: C₁₀H₁₁NO₂

Molecular Weight: 177.202

Accurate Mass: 177.078979

Percentage Composition: C 67.78%; H 6.26%; N 7.90%; O 18.06%

Use/Importance: Chiral reagent and auxiliary

Physical Description: Needles (EtOAc/hexane)

Melting Point: Mp 87-88.5°

Optical Rotation: [α]_D+4.9 (c, 1.1 in EtOH). [α]_D²⁵-62 (c, 1 in CHCl₃) (>99% ee)

Aldrich: 29464-0

Fluka: 13616

Sigma: B2018

>>Derivative: *N*-Ac

CAS Registry Number: 132836-66-9

Molecular Formula: C₁₂H₁₃NO₃

Molecular Weight: 219.24

Accurate Mass: 219.089544

Percentage Composition: C 65.74%; H 5.98%; N 6.39%; O 21.89%

Use/Importance: Recyclable chiral auxiliary for aldol condensations, Diels-Alder cycloaddition and other reactions

Melting Point: Mp 104-106°

Optical Rotation: [α]_D²⁰+110 (c, 1 in CHCl₃)

>>Derivative: *N*-Chloroacetyl

CAS Registry Number: 104324-16-5

Molecular Formula: C₁₂H₁₂ClNO₃

Molecular Weight: 253.684

Accurate Mass: 253.050571

Percentage Composition: C 56.82%; H 4.77%; Cl 13.98%; N 5.52%; O 18.92%

Melting Point: Mp 172-174°

Optical Rotation: [α]_D²⁰+49 (c, 2 in CHCl₃)