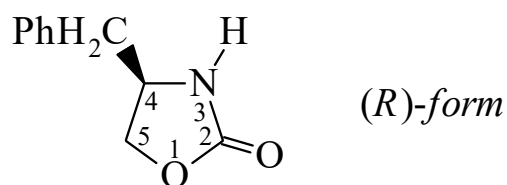




>>Entry Name: 4-Benzyl-2-oxazolidinone, 8Cl
Synonym(s): 4-(Phenylmethyl)-2-oxazolidinone, 9Cl



CAS Registry Number: 40217-17-2

Molecular Formula: $C_{10}H_{11}NO_2$

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: $C_{10}H_{11}NO_2$

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: $[\alpha]_D^{25} +64$ (c, 1 in $CHCl_3$)

Aldrich: 30097-7

Fluka: 13615

Sigma: B7268

>>Variant: (*S*)-form

CAS Registry Number: 90719-32-7

Molecular Formula: $C_{10}H_{11}NO_2$

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: $[\alpha]_D +4.9$ (c, 1.1 in EtOH). $[\alpha]_D^{25} -62$ (c, 1 in $CHCl_3$) (>99% ee)

Aldrich: 29464-0

Fluka: 13616

Sigma: B2018

>>Derivative: *N*-Ac

CAS Registry Number: 132836-66-9

Molecular Formula: $C_{12}H_{13}NO_3$

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: $[\alpha]_D^{20} +110$ (c, 1 in $CHCl_3$)

>>Derivative: *N*-Chloroacetyl

CAS Registry Number: 104324-16-5

Molecular Formula: $C_{12}H_{12}ClNO_3$

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: $[\alpha]_D^{20} +49$ (c, 2 in $CHCl_3$)