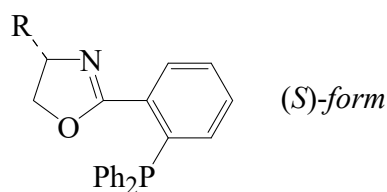




>>Entry Name: 4-Alkyl-2-[2-(diphenylphosphino)phenyl]-4,5-dihydrooxazoles

Synonym(s): 4-Alkyl-2-[2-(diphenylphosphino)phenyl]-2-oxazolines



Related CAS Registry Numbers(s): 164858-78-0 164858-79-1 167171-03-1

Use/Importance: Chiral ligands used in metal-catalysed enantioselective reactions incl. allylic substitution, Heck reactions and hydrogenations

Other Data: Props. given refer to the (S)-enantiomers illus.

>>Variant: 2-[2-(Diphenylphosphino)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole, 9Cl

Synonym(s): 2-[2-(Diphenylphosphino)phenyl]-4-isopropyl-2-oxazoline

CAS Registry Number: 148461-14-7

Molecular Formula: C₂₄H₂₄NOP

Molecular Weight: 373.434

Accurate Mass: 373.159551

Percentage Composition: C 77.19%; H 6.48%; N 3.75%; O 4.28%; P 8.29%

Use/Importance: Chiral ligand

Physical Description: Needles

Melting Point: Mp 84-85°

Optical Rotation: $[\alpha]_{\text{D}}^{23}$ -44.9 (c, 1.40 in CHCl₃)

>>Variant: 4-(1,1-Dimethylethyl)-2-[2-(diphenylphosphino)phenyl]-4,5-dihydrooxazole, 9Cl

Synonym(s): 4-*tert*-Butyl-2-[2-(diphenylphosphino)phenyl]-2-oxazoline

CAS Registry Number: 148461-16-9

Extra CAS Registry Numbers(s): 151644-44-9

Molecular Formula: C₂₅H₂₆NOP

Molecular Weight: 387.46

Accurate Mass: 387.175201

Percentage Composition: C 77.50%; H 6.76%; N 3.62%; O 4.13%; P 7.99%

Use/Importance: Chiral ligand

Physical Description: Needles

Melting Point: Mp 114-115°

Optical Rotation: $[\alpha]_{\text{D}}^{20}$ -61.9 (c, 1.755 in CHCl₃)

>>Variant: 2-[2-(Diphenylphosphino)phenyl]-4,5-dihydro-4-(phenylmethyl)oxazole, 9Cl

Synonym(s): 4-Benzyl-2-[2-(diphenylphosphino)phenyl]-2-oxazoline

CAS Registry Number: 148461-13-6

Molecular Formula: C₂₈H₂₄NOP

Molecular Weight: 421.478

Accurate Mass: 421.159551

Percentage Composition: C 79.79%; H 5.74%; N 3.32%; O 3.80%; P 7.35%

Use/Importance: Chiral ligand

Physical Description: Solid

Melting Point: Mp 106-108°

Optical Rotation: $[\alpha]_{\text{D}}^{23}$ +25.8 (c, 1.1 in CHCl₃)

>>Variant: 2-[2-(Diphenylphosphino)phenyl]-4,5-dihydro-4-phenyloxazole, 9Cl

Synonym(s): 2-[2-(Diphenylphosphino)phenyl]-4-phenyl-2-oxazoline

CAS Registry Number: 148461-15-8

Extra CAS Registry Numbers(s): 189169-55-9

Molecular Formula: C₂₇H₂₂NOP

Molecular Weight: 407.451

Accurate Mass: 407.143901

Percentage Composition: C 79.59%; H 5.44%; N 3.44%; O 3.93%; P 7.60%

Use/Importance: Chiral ligand

Physical Description: Solid

Melting Point: Mp 57-58°

Optical Rotation: $[\alpha]$