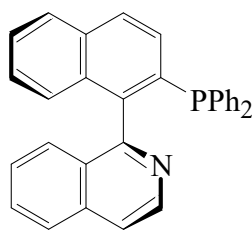




>>Entry Name: 1-[2-(Diphenylphosphino)-1-naphthalenyl]isoquinoline, 9Cl

Synonym(s): 2-Diphenylphosphino-1-isoquinolinyl-naphthalene. (1-Isoquinolinyl-2-naphthalenyl)diphenylphosphine



(*S*<sub>ax</sub>)-form

Type of Compound Code(s): AC0300

Molecular Formula: C<sub>31</sub>H<sub>22</sub>NP

Molecular Weight: 439.495

Accurate Mass: 439.148986

Percentage Composition: C 84.72%; H 5.05%; N 3.19%; P 7.05%

General Statement: Atropisomeric ligand

Use/Importance: Pd complex used as catalyst in allylic alkylations

>>Variant: (*R*<sub>ax</sub>)-form

CAS Registry Number: 149341-34-4

Type of Compound Code(s): AC0300

Molecular Formula: C<sub>31</sub>H<sub>22</sub>NP

Molecular Weight: 439.495

Accurate Mass: 439.148986

Percentage Composition: C 84.72%; H 5.05%; N 3.19%; P 7.05%

Physical Description: Solid

Optical Rotation: [ $\alpha$ ]<sub>D</sub><sup>21</sup>+153.2 (c, 1.0 in CHCl<sub>3</sub>)

>>Variant: (*S*<sub>ax</sub>)-form

CAS Registry Number: 149341-33-3

Type of Compound Code(s): AC0300

Molecular Formula: C<sub>31</sub>H<sub>22</sub>NP

Molecular Weight: 439.495

Accurate Mass: 439.148986

Percentage Composition: C 84.72%; H 5.05%; N 3.19%; P 7.05%

Physical Description: Solid

Melting Point: Mp 226-231°

Optical Rotation: [ $\alpha$ ]<sub>D</sub><sup>21</sup>-153 (c, 1.0 in CHCl<sub>3</sub>)

>>Variant: ( $\pm$ )-form

CAS Registry Number: 149245-03-4

Type of Compound Code(s): AC0300

Molecular Formula: C<sub>31</sub>H<sub>22</sub>NP

Molecular Weight: 439.495

Accurate Mass: 439.148986

Percentage Composition: C 84.72%; H 5.05%; N 3.19%; P 7.05%

General Statement: Resolved through a Pd complex

Physical Description: Cryst. (CH<sub>2</sub>Cl<sub>2</sub>)

Melting Point: Mp 217-219°

>>Derivative: *P*-Oxide

CAS Registry Number: 149245-07-8

Type of Compound Code(s): AC0310

Molecular Formula: C<sub>31</sub>H<sub>22</sub>NOP

Molecular Weight: 455.495

Accurate Mass: 455.143901

Percentage Composition: C 81.74%; H 4.87%; N 3.08%; O 3.51%; P 6.80%

Physical Description: Fine powder (toluene)

Melting Point: Mp 215-218°

References: