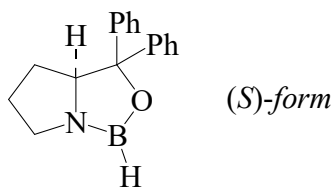




>>Entry Name: Tetrahydro-3,3-diphenyl-1*H*,3*H*-pyrrolo[1,2-*c*][1,3,2]oxazaborole
ENTRY UNDER REVIEW



Related CAS Registry Numbers(s): 112022-83-0 121944-12-5 133261-83-3 141197-93-5

Molecular Formula: C₁₇H₁₈BNO

Molecular Weight: 263.146

Accurate Mass: 263.148144

Percentage Composition: C 77.59%; H 6.89%; B 4.11%; N 5.32%; O 6.08%

>>Variant: (*S*)-form

CAS Registry Number: 110205-59-9

Molecular Formula: C₁₇H₁₈BNO

Molecular Weight: 263.146

Accurate Mass: 263.148144

Percentage Composition: C 77.59%; H 6.89%; B 4.11%; N 5.32%; O 6.08%

Use/Importance: Catalyst for enantioselective ketone redn.

Physical Description: Cryst. (THF or by subl.)

Melting Point: Mp 107-124°

Boiling Point: Bp_{0.05} 145-160° subl.

Solubility: Sol. THF

Other Data: Ir ν_{B-H} 2568 cm⁻¹(THF)

>>Derivative: Dimer

Molecular Formula: C₃₄H₃₆B₂N₂O₂

Molecular Weight: 526.293

Accurate Mass: 526.296288

Percentage Composition: C 77.59%; H 6.89%; B 4.11%; N 5.32%; O 6.08%

Other Data: Ir ν_{B-H} 2413 cm⁻¹

>>Derivative: *B*-Me

Synonym(s): Tetrahydro-1-methyl-3,3-diphenyl-1*H*,3*H*-pyrrolo[1,2-*c*][1,3,2]oxazaborole. Corey catalyst. Me CBS

CAS Registry Number: 112022-81-8

Source/Synthesis: Synth. from (*S*)-diphenylprolinol + trimethylboroxine

Use/Importance: Catalyst for enantioselective redn. of ketones by BH₃

Physical Description: Solid

Melting Point: Mp 79-81°

Other Data: (*R*)-isomer also known

Aldrich: 45770-1

Other: Callery

>>Derivative: *B*-Butyl

CAS Registry Number: 129145-37-5

Molecular Formula: C₂₁H₂₆BNO

Molecular Weight: 319.254

Accurate Mass: 319.210744

Percentage Composition: C 79.01%; H 8.21%; B 3.39%; N 4.39%; O 5.01%

Source/Synthesis: Synth. from (*S*)-diphenylprolinol + tributylboroxine

Use/Importance: Catalyst for enantioselective redn. of ketones by BH₃

Physical Description: Oil