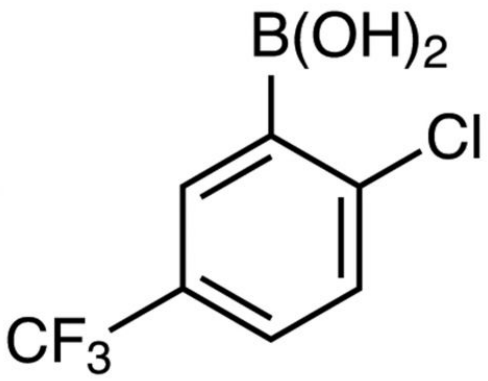
Product Data Sheet

Product Name: 2-Chloro-5-(trifluoromethyl)benzeneboronic acid
Cat. No.: GD05924

Chemical Properties

Cas. No.	182344-18-9		
Formula	$C_7H_5BClF_3O_2$	M.Wt	224.373
Solubility		Storage	Store at RT
General tips	For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20°C for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure			



Protocol

Application of 2-Chloro-5-(trifluoromethyl)benzeneboronic acid in Suzuki-Miyaura Coupling Reaction[1]

This protocol is adapted from research data and provided for reference only. Adjustments may be necessary based on specific experimental requirements.

1. Reagent Preparation: Weigh 8-Bromo-4H-[1,2,4]oxadiazolo[3,4-c][1,4]benzoxazin-1-one (NS2028) and 2-Chloro-5-(trifluoromethyl)benzeneboronic acid at a molar ratio of 1:2 for later use. Weigh

$Pd(OAc)_2$ as the catalyst, using 10mol% relative to the molar amount of NS2028. Weigh KOAc as the base. Prepare anhydrous MeCN, distilled from calcium hydride and stored over 4Å molecular sieves, as the reaction solvent.

2. Reaction Setup: Place NS2028, 2-Chloro-5-(trifluoromethyl)benzeneboronic acid, KOAc, and $Pd(OAc)_2$ into a thick-walled glass reaction tube. Add anhydrous acetonitrile to dissolve. Seal the reaction tube.

3. Reaction Execution: Heat the sealed reaction tube at approximately 110°C for 12 hours, then cool to room temperature (approximately 20°C).

4. Product Isolation and Purification: Remove the volatile solvents under reduced pressure. Dissolve the residue in dichloromethane (DCM) and load it onto silica gel. Purify using dry flash chromatography with DCM as the eluent. The by-product, 2,2'-dichloro-5,5'-bis(trifluoromethyl)-1,1'-biphenyl, is eluted first. Continued elution yields the target product, 8-[2-Chloro-5-(trifluoromethyl)phenyl]-4H-[1,2,4]oxadiazolo[3,4-c][1,4]benzoxazin-1-one.

Precautions:

(1) This reaction must be carried out in a sealed tube under strictly anhydrous conditions. The use of anhydrous solvents and reagents is crucial for the success of the reaction.

(2) Perform the operation inside a fume hood.

(3) For your safety and health, please wear a lab coat and disposable gloves during operation.

References:
[1] Berezin, Andrey A, P. Koutentis. 8-(2-Chloro-5-(trifluoromethyl)phenyl)-4H-(1,2,4)oxadiazolo- (3,4-c)(1,4)benzoxazin-1-one. Molbank. 2011 (2011).

Background

2-Chloro-5-(trifluoromethyl)benzeneboronic acid can serve as a reagent and intermediate in Suzuki coupling reactions to participate in carbon-carbon bond formation. 2-Chloro-5-(trifluoromethyl)benzeneboronic acid can also act as a boronic acid catalyst ligand in organic reactions such as olefin boronic acid isomerization[1].

References:

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[1] Berezin, Andrey A, P. Koutentis. 8-(2-Chloro-5-(trifluoromethyl)phenyl)-4H-(1,2,4)oxadiazolo- (3,4-c)(1,4)benzoxazin-1-one. Molbank. 2011 (2011).

Caution: Product has not been fully validated for medical applications. For research use only.
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