Product Data Sheet

Product Name: 4-(n-nonyl) Benzeneboronic Acid
Cat. No.: GC17159

Chemical Properties

Cas. No.	256383-45-6		
Chemical Name	B-(4-nonylphenyl)-boronic acid		
SMILES	CCCCCCCCCC1=CC=C(B(O)O)C=C1		
Formula	$C_{15}H_{25}BO_2$	M.Wt	248.2
Solubility	≥ 11.75mg/mL in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ 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			

Background

IC50: 9.1 nM

4-(n-nonyl) Benzeneboronic acid is a dual FAAH inhibitor.

Fatty acid amide hydrolase (FAAH), a membrane-bound enzyme of the endocannabinoid system, has been identified as a potential target for therapeutic agents in the treatment of various medical conditions, such as inflammation and pain. FAAH and monoglyceride lipase (MGL) have been reported to be the primary enzyme responsible for the hydrolysis of endocannabinoid N-arachidonoyl ethanolamide (AEA), which is a key lipid messenger in the brain and periphery.

In vitro: 4-(n-Nonyl) benzeneboronic acid was synthezed as a potent inhibitor of FAAH, with an IC50 of 9.1 nM. 4-(n-Nonyl) benzeneboronic acid was also found to be able to inhibit MAGL, which could hydrolyze 2-arachidonoyl glycerol, but at around 1000-fold higher concentration. Moreover, it was found that as the most potent para-substituted

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compound, 4-(n-Nonyl) benzeneboronic acid showed rather high pKa of 9.1. In addition, the molecular docking was utilized to gain insight on the FAAH binding mode of 4-(n-Nonyl) benzeneboronic acid and a putative binding mode was observed [1].

In vivo: Up to now, there is no animal in vivo data reported.

Clinical trial: So far, no clinical study has been conducted.

Reference:
[1] Minkkil, A. ,Saario, S.M.,Ksnnen, H., et al. Discovery of boronic acids as novel and potent inhibitors of fatty acid amide hydrolase. Journal of Medicinal Chemistry 51, 7057-7060 (2008).