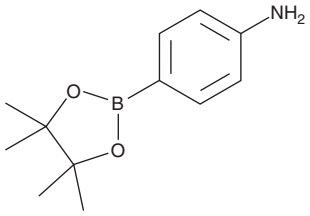
PRODUCT INFORMATION

4-(4,4,5,5-Tetramethyl-1,3,2-dioxaboran-2yl)aniline

Item No. 30402

CAS Registry No.: 214360-73-3
Formal Name: 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-benzenamine
Synonym: 4-Aminophenylboronic Acid pinacol ester
MF: $C_{12}H_{18}BNO_2$
FW: 219.1
Purity: ≥98%
UV/Vis.: λ_{max}: 262 nm
Supplied as: A solid
Storage: -20°C
Stability: ≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

4-(4,4,5,5-Tetramethyl-1,3,2-dioxaboran-2yl)aniline is supplied as a solid. A stock solution may be made by dissolving the 4-(4,4,5,5-tetramethyl-1,3,2-dioxaboran-2yl)aniline in the solvent of choice, which should be purged with an inert gas. 4-(4,4,5,5-Tetramethyl-1,3,2-dioxaboran-2yl)aniline is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of 4-(4,4,5,5-tetramethyl-1,3,2-dioxaboran-2yl)aniline in these solvents is approximately 3, 10, and 20 mg/ml, respectively.

4-(4,4,5,5-Tetramethyl-1,3,2-dioxaboran-2yl)aniline is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, 4-(4,4,5,5-tetramethyl-1,3,2-dioxaboran-2yl)aniline should first be dissolved in DMF and then diluted with the aqueous buffer of choice. 4-(4,4,5,5-Tetramethyl-1,3,2-dioxaboran-2yl) aniline has a solubility of approximately 0.16 mg/ml in a 1:5 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

4-(4,4,5,5-Tetramethyl-1,3,2-dioxaboran-2yl)aniline is a heterocyclic building block.[1,2] It has been used in the synthesis of 3-aminoindazole-based multi-targeted receptor tyrosine kinase (RTK) inhibitors with anticancer activity and roscovitine derivatives that are dual inhibitors of cyclin-dependent kinases (CDKs) and casein kinase 1 (CK1).

References

1. Dai, Y., Hartandi, K., Ji, Z., *et al.* Discovery of *N*-(4-(3-amino-1*H*-indazol-4-yl)phenyl)-*N'*-(2-fluoro-5-methylphenyl)urea (ABT-869), a 3-aminoindazole-based orally active multitargeted receptor tyrosine kinase inhibitor. *J. Med. Chem.* **50(7)**, 1584-1597 (2007).
2. Paraiso, K.H.T., Haarberg, H.E., Wood, E., *et al.* The HSP90 inhibitor XL888 overcomes BRAF inhibitor resistance mediated through diverse mechanisms. *Clin. Cancer Res.* **18(9)**, 2502-2514 (2012).

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