# Data Sheet

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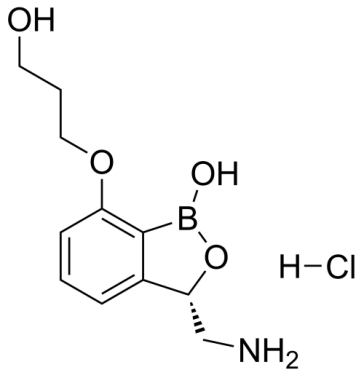
| **Product Name:** | Epetraborole (hydrochloride) |
| **Cat. No.:** | CS-5750 |
| **CAS No.:** | 1234563-16-6 |
| **Molecular Formula:** | $C_{11}H_{17}BClNO_4$ |
| **Molecular Weight:** | 273.52 |
| **Target:** | Aminoacyl-tRNA Synthetase; Bacterial |
| **Pathway:** | Anti-infection; Metabolic Enzyme/Protease |
| **Solubility:** | DMSO : 200 mg/mL (731.21 mM; Need ultrasonic); H2O : ≥ 28 mg/mL (102.37 mM) |




## BIOLOGICAL ACTIVITY:

Epetraborole (GSK2251052) hydrochloride is a novel **leucyl-tRNA synthetase** (**LeuRS**) inhibitor (**$IC_{50}$**=0.31 μM), thereby inhibiting protein synthesis. Epetraborole hydrochloride can be used in multidrug-resistant gram-negative pathogens infection research[1][2][3]. IC50 & Target:$IC_{50}$: 0.31 μM (LeuRS)[3] **In Vitro:**Epetraborole (0-32 μg/mL) shows anti-bacterial activity against key gram-negative aerobic and anaerobic pathogens and gram-positive anaerobes[1].

## References:

[1]. Goldstein EJ, et al. Comparative in vitro activities of GSK2251052, a novel boron-containing leucyl-tRNA synthetase inhibitor, against 916 anaerobic organisms. Antimicrob Agents Chemother. 2013 May;57(5):2401-4.

[2]. O'Dwyer K, et al. Bacterial resistance to leucyl-tRNA synthetase inhibitor GSK2251052 develops during treatment of complicated urinary tract infections. Antimicrob Agents Chemother. 2015 Jan;59(1):289-98.

[3]. Sutcliffe JA. Antibiotics in development targeting protein synthesis. Ann N Y Acad Sci. 2011 Dec;1241:122-52.

## CAIndexNames:

1-Propanol, 3-[[(3S)-3-(aminomethyl)-1,3-dihydro-1-hydroxy-2,1-benzoxaborol-7-yl]oxy]-, hydrochloride (1:1)

## SMILES:

OCCCOC1=C(B(O)O[C@@H]2CN)C2=CC=C1.[H]Cl



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