

# PRODUCT INFORMATION

## 3,6-dichloro-benzo[b]thiophene-2-Carboxylic Acid

Item No. 22948

CAS Registry No.: 34576-94-8

Formal Name: 3,6-dichloro-benzo[b]thiophene-2-carboxylic acid

MF: C<sub>9</sub>H<sub>4</sub>Cl<sub>2</sub>O<sub>2</sub>S

FW: 247.1

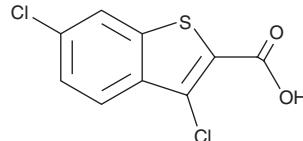
Purity: ≥95%

UV/Vis.:  $\lambda_{\text{max}}$ : 239, 251, 296 nm

Supplied as: A crystalline 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

3,6-dichloro-benzo[b]thiophene-2-Carboxylic acid is supplied as a crystalline solid. A stock solution may be made by dissolving the 3,6-dichloro-benzo[b]thiophene-2-carboxylic acid in the solvent of choice. 3,6-dichloro-benzo[b]thiophene-2-Carboxylic acid is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of 3,6-dichloro-benzo[b]thiophene-2-carboxylic acid in ethanol is approximately 1 mg/ml and approximately 30 mg/ml in DMSO and DMF.

### Description

3,6-dichloro-benzo[b]thiophene-2-Carboxylic acid is an inhibitor of myeloid cell leukemia 1 (Mcl-1) with a K<sub>i</sub> value of 59  $\mu$ M for binding of FITC-Mcl-1-BH2 peptide binding to Mcl-1.<sup>1</sup> It has been used as a building block in the synthesis of inhibitors of Mcl-1, the toll-like receptor 3/double-stranded RNA (TLR3/dsRNA) complex, and D-amino acid oxidase (DAO).<sup>1-3</sup>

### References

1. Friberg, A., Vigil, D., Zhao, B., et al. Discovery of potent myeloid cell leukemia 1 (Mcl-1) inhibitors using fragment-based methods and structure-based design. *J. Med Chem.* **56**(1), 15-30 (2013).
2. Cheng, K., Wang, X., and Yin, H. Small-molecule inhibitors of the TLR3/dsRNA complex. *J. Am. Chem. Soc.* **133**(11), 3764-3767 (2011).
3. Katane, M., Osaka, N., Matsuda, S., et al. Identification of novel D-amino acid oxidase inhibitors by in silico screening and their functional characterization in vitro. *J. Med Chem.* **56**(5), 1894-1907 (2013).

#### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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