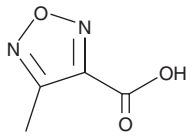
PRODUCT INFORMATION

4-Methyl-1,2,5-oxadiazole-3-carboxylic Acid

Item No. 46443

CAS Registry No.: 58677-34-2
Synonym: NSC 234497
MF: $C_4H_4N_2O_3$
FW: 128.1
Purity: ≥98%
Supplied as: A solid
Storage: -20°C
Stability: ≥4 years



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

Laboratory Procedures

4-Methyl-1,2,5-oxadiazole-3-carboxylic acid is supplied as a solid. A stock solution may be made by dissolving the 4-methyl-1,2,5-oxadiazole-3-carboxylic acid in the solvent of choice, which should be purged with an inert gas. 4-Methyl-1,2,5-oxadiazole-3-carboxylic acid is soluble (≥10 mg/ml) in ethanol and DMSO.

Further dilutions of the stock solution into aqueous buffers or isotonic saline should be made prior to performing biological experiments. Ensure that the residual amount of organic solvent is insignificant, since organic solvents may have physiological effects at low concentrations. Organic solvent-free aqueous solutions of 4-methyl-1,2,5-oxadiazole-3-carboxylic acid can be prepared by directly dissolving the solid in aqueous buffers. 4-Methyl-1,2,5-oxadiazole-3-carboxylic acid is soluble (≥10 mg/ml) in PBS (pH 7.2). We do not recommend storing the aqueous solution for more than one day.

Description

4-Methyl-1,2,5-oxadiazole-3-carboxylic acid is a synthetic intermediate.[1-3] It has been used in the synthesis of compounds with anti-inflammatory or anti-tuberculosis activity.[2,3]

References

1. Yang, Q., Lu, Y., Xia, H., *et al.* Safety guided process development and scale-up of the highly energetic compound 4-methyl-1,2,5-oxadiazole-3-carboxylic acid. *Org. Process Res. Dev.* **28(7)**, 2794-2805 (2024).
2. Yang, Q., Linder, R.J., Lu, Y., *et al.* Development of a scalable process for an IL-17A inhibitor LY3509754: Part III. Assembly of drug substance, salt formation, and impurity control. *Org. Process Res. Dev.* **29(4)**, 1019-1035 (2025).
3. Guo, S., Song, Y., Huang, Q., *et al.* Identification, synthesis, and pharmacological evaluation of tetrahydroindazole based ligands as novel antituberculosis agents. *J. Med. Chem.* **53(2)**, 649-659 (2010).

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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