

## Product Data Sheet

Product Name: SIN-1 chloride

Cat. No.: GC13152

### Chemical Properties

Cas. No. 16142-27-1

Chemical Name 5-imino-3-morpholino-5H-1,2,3-oxadiazol-3-ium-2-ide hydrochloride

SMILES N=C1C=N(N2CCOCC2)=NO1.Cl

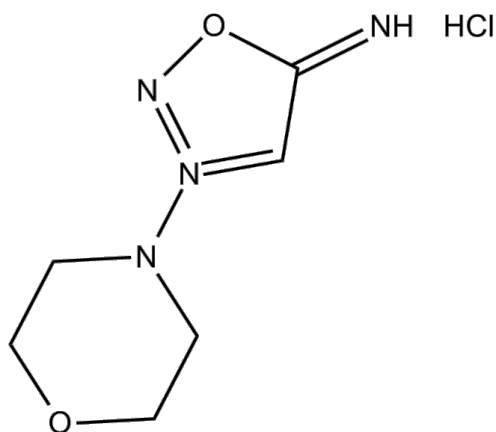
Formula  $C_6H_{11}ClN_4O_2$  M.Wt 206.63

Solubility >9 mg/ml in DMSO, >5 mg/ml in DMF, >8 mg/ml in Ethanol Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C 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

As the active metabolite of molsidomine, SIN-1 (chloride) is a potent vasorelaxant and inhibitor of platelet aggregation. It produces both NO and superoxide and can therefore be used to generate peroxynitrite under physiological conditions.

SIN-1 (chloride) is supplied as a crystalline solid. A stock solution may be made by dissolving the

**Caution: Product has not been fully validated for medical applications. For research use only.**

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SIN-1 (chloride) in an organic solvent. SIN-1 (chloride) is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of SIN-1 (chloride) in these solvents is approximately 5 mg/ml.

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 SIN-1 (chloride) can be prepared by directly dissolving the crystalline compound in aqueous buffers. The solubility of SIN-1 (chloride) in PBS (pH 7.2) is approximately 10 mg/ml. We do not recommend storing the aqueous solution for more than one day.

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**WARNING** This product is not for human or veterinary use.

### References:

1. Rosenkranz, B, Winkelmann, B.R., and Parnham, M.J. Clinical pharmacokinetics of molsidomine. Clin. Pharmacokinet. 30, 372-384 (1996).
2. Lomonosova, E.E, Kirsch, M, Rauen, U, et al. The critical role of hemes in SIN-1 cytotoxicity, peroxynitrite versus hydrogen peroxide. Free Radic. Biol Med. 24, 522-528 (1998).
3. Nishikawa, M., Kanamori, M., and Hidaka, H. Inhibition of platelet aggregation and stimulation of guanylate cyclase by an antianginal agent molsidomine and its metabolites. J. Pharmacol. Exp. Ther. 220, 183-190 (1982).

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