Data Sheet (Cat.No.T67058)

TargetMol

Chlorobutanol hemihydrate

Chemical Properties

CAS No. :	6001-64-5
Formula:	C4H7Cl3O 1/2H2O
Molecular Weight:	186.46
Storage:	Keep away from moisture Powder: -20°C for 3 years | In solvent: -80°C for 1 year Actual storage temperature shall be subject to the COA.

Biological Description

Description	Chlorobutanol hemihydrate (Chlorbutol hemihydrate) is an orally toxic preservative with antimicrobial activity that inhibits Gram-positive and Gram-negative bacteria and fungi, inhibits the aggregation and release of human platelets in vitro, and is commonly used in cosmetics.
Targets(IC50)	Antibacterial,Antibiotic,Antifungal
In vivo	The high dose was set at 100 mg/kg/day and the medium, medium-low, and low doses were set at 50 mg/kg/day, 25 mg/kg/day, and 12.5 mg/kg/day, respectively, in a 28-day repeated-dose toxicity study by gavage.There was no significant change in body weight in the repeated-dose toxicity study.100 mg/kg/day The relative weights of liver and kidney were significantly increased in both sexes in the dose group.[1]

Solubility Information

Solubility	DMSO: 80 mg/mL(429.05 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (10.73 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	5.3631 mL	26.8154 mL	53.6308 mL
5 mM	1.0726 mL	5.3631 mL	10.7262 mL
10 mM	0.5363 mL	2.6815 mL	5.3631 mL
50 mM	0.1073 mL	0.5363 mL	1.0726 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Jeong D, et al. In Vivo Evaluation of the Oral Toxicity of the Chlorobutanol. Toxics. 2022 Jan 7;10(1):24.
Smoak IW, et al. Chlorobutanol: maternal serum levels and placental transfer in the mouse. Vet Hum Toxicol. 1997 Oct;39(5):287-90.
Habara Y, et al. Dual effects of chlorobutanol on secretory response and intracellular Ca2+ dynamics in isolated pancreatic acini of the rat. Br J Pharmacol. 1993 Jul;109(3):685-92.