

5-Chlorovaleronitrile

Chemical Properties

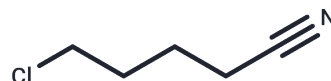
CAS No. : 6280-87-1

Formula: C₅H₈ClN

Molecular Weight: 117.58

Storage: Pure form: -20°C for 3 years | In solvent: -80°C for 1 year

Actual storage temperature shall be subject to the COA.



Biological Description

Description	5-Chlorovaleronitrile (A1320151) can be used as a quantitative structure-toxicity model to predict the aquatic toxicity.
Targets(IC50)	Others

Solubility Information

Solubility	DMSO: 55 mg/mL (467.77 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	8.5048 mL	42.5242 mL	85.0485 mL
5 mM	1.701 mL	8.5048 mL	17.0097 mL
10 mM	0.8505 mL	4.2524 mL	8.5048 mL
50 mM	0.1701 mL	0.8505 mL	1.701 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

Polishchuk PG, et al. Application of random forest approach to QSAR prediction of aquatic toxicity. J Chem Inf Model. 2009 Nov;49(11):2481-8.

Toropov AA, Schultz TW. Prediction of aquatic toxicity: use of optimization of correlation weights of local graph invariants. J Chem Inf Comput Sci. 2003 Mar-Apr;43(2):560-7.

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