

Product Data Sheet

Product Name: 2-cyano-Pyrimidine

Cat. No.: GC11553

Chemical Properties

Cas. No. 14080-23-0

Chemical Name 2-pyrimidinecarbonitrile

SMILES NCc1ncccc1

Formula $C_5H_3N_3$

M.Wt 124.1

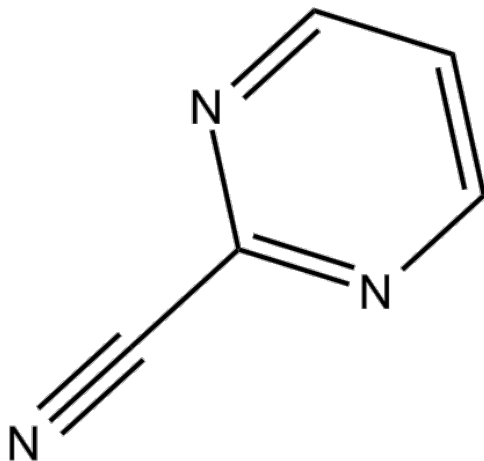
Solubility DMF: 30 mg/ml, DMSO: 30 mg/ml, Ethanol: 20 mg/ml, PBS (pH 7.2): 3 mg/ml

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

IC50: 170 nM

2-cyano-Pyrimidine is a cathepsin K inhibitor.

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

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Cathepsin K is a protease defined by its high specificity for kinins, which is involved in bone resorption. Cathepsin K's ability to catabolize collagen, elastin, and gelatin allow it to break down bone and cartilage. Such catabolic activity is also partially responsible for the loss of lung elasticity and recoil in emphysema. Therefore, inhibitors of Cathepsin K are showing great potential in the treatment of osteoporosis.

In vitro: 2-cyano-Pyrimidine was identified as a cathepsin K inhibitor whose basic structure and derivatives have been evaluated for the treatment of osteoporosis. Enzymatic study showed that 2-cyano-Pyrimidine had an IC₅₀ value of 170 nM for inhibition of cathepsin K, elevated activity of which has been linked to the formation of osteoporosis and arthritis. Moreover, Cathepsin K was found to be a lysosomal cysteine protease found in osteoclasts. [1,2].

In vivo: Up to now, there is no animal in vivo data reported.

Clinical trial: So far, no clinical study has been conducted.

References:

- [1] Altmann, E., Aichholz, R., Betschart, C., et al. 2-cyano-pyrimidines: A new chemotype for inhibitors of the cysteine protease cathepsin K. Journal of Medicinal Chemistry 50(4), 591-594 (2007).
- [2] Rankovic Z et al. Design and optimization of a series of novel 2-cyano-pyrimidines as cathepsin K inhibitors. Bioorg Med Chem Lett. 2010 Mar 1;20(5):1524-7.

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