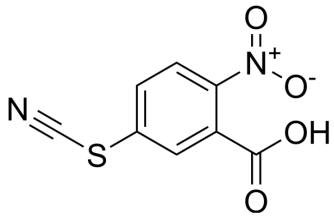
2-Nitro-5-thiocyanatobenzoic acid

Cat. No.:	HY-137541
CAS No.:	30211-77-9
Molecular Formula:	$C_8H_4N_2O_4S$
Molecular Weight:	224.19
Target:	Biochemical Assay Reagents
Pathway:	Others
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (446.05 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	4.4605 mL	22.3025 mL	44.6050 mL
	5 mM	0.8921 mL	4.4605 mL	8.9210 mL
	10 mM	0.4461 mL	2.2303 mL	4.4605 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (11.15 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (11.15 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (11.15 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

2-Nitro-5-thiocyanatobenzoic acid (NTCB) is a highly reactive reagent that transfers its cyano group rapidly to a nucleophilic thiolate. 2-Nitro-5-thiocyanatobenzoic acid has been proposed as a reagent for converting thiol groups in proteins into their S-cyano derivatives[1][2].

In Vitro

2-Nitro-5-thiocyanatobenzoic acid NTCB is a highly reactive reagent that transfers its cyano group rapidly to a nucleophilic thiolate. When it is provided to a protein, it will quickly cyanylate the protein cysteine to form S-cyano-cysteine which undergoes reversible intramolecular addition with the cysteine N-amide to generate 1-acyl-2-iminothiazolidine, an

intermediate that can undergo nucleophilic acyl substitution[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Qiao Y, et al. Site-Specific Conversion of Cysteine in a Protein to Dehydroalanine Using 2-Nitro-5-thiocyanatobenzoic Acid. Molecules. 2021;26(9):2619. Published 2021 Apr 29.

[2]. Price NC. Alternative products in the reaction of 2-nitro-5-thiocyanatobenzoic acid with thiol groups. Biochem J. 1976;159(1):177-180.

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