Product Data Sheet

Product Name: 2,3-dihydrothieno-Thiadiazole Carboxylate
Cat. No.: GC13836

Chemical Properties

Cas. No.	152467-47-5		
Chemical Name	methylthieno[3,2-d][1,2,3]thiadiazole-6-carboxylate		
SMILES	O=C(OC)C1=CSC2=C1N=NS2		
Formula	$C_6H_4N_2O_2S_2$	M.Wt	200.2
Solubility	≤2mg/ml in ethanol;30mg/ml in DMSO;30mg/ml in dimethyl formamide	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ 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

2,3-dihydrothieno-Thiadiazole Carboxylate is a CYP450 (CYP2E1 and CYP2B4) inhibitor.

The cytochrome P450 (CYP) enzymes are a superfamily of oxidative catalysts critical in the biosynthesis and metabolism of various endobiotics such as steroids and steroid hormones, the neurotransmitter nitric oxide, and vitamins A and D. The cytochrome P450 enzymes are also involved in the metabolism of xenobiotics including natural products, drugs, and other organic chemicals.

In vitro: As a 1,2,3-thiadiazole analog, 2,3-dihydrothieno-thiadiazole carboxylate could both inhibit and inactivate certain microsomal CYP450 enzymes (CYP2E1 and CYP2B4) at 100 μM, but not others (CYP1A2). Moreover, P450 2E1 was significantly more sensitive than P450 2B4 to mechanism-based inactivation by 2,3-dihydrothieno-thiadiazole carboxylate when compared by the difference in partition numbers and inactivation rate constants. Inactivation rate constants (kinact) determined from plots of 1/kobs versus

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com
Address: 10292 Central Ave. #205, Montclair, CA, USA

Product Data Sheet

1/[I] were 0.08 for 2E1 and 0.04 min-1 for P450 2B4, with Kis of 0.1 and 2.0 mM, respectively. The difference in the oxidation of the monocyclic and bicyclic thaidiazoles might account for the ability of 2,3-dihydrothieno-thiadiazole carboxylate to function as a mechanism-based inactivator [1].

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

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

Reference:
[1] Babu, B. R. and Vaz, A.D.N. 1,2,3-thiadiazole: A novel heterocyclic heme ligand for the design of cytochrome P450 inhibitors. Biochemistry 36, 7209-7216 (1997).

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com
Address: 10292 Central Ave. #205, Montclair, CA, USA