
Product Data Sheet

Product Name: 4-phenyl-5-methyl-1,2,3-Thiadiazole

Cat. No.: GC11758

Chemical Properties

Cas. No. 64273-28-5

Chemical Name 5-methyl-4-phenyl-1,2,3-thiadiazole

SMILES Cc1snnc1c1ccccc1

Formula $C_9H_8N_2S$

M.Wt 176.2

Solubility $\geq 7.85\text{mg/mL}$ in DMSO

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

4-phenyl-5-methyl-1,2,3-Thiadiazole is a CYP2B4 and CYP2E1 inhibitor.

Cytochrome P450 (CYP450) enzymes, a superfamily of oxidative catalysts, are important in the biosynthesis and metabolism of a wide range of endogenous molecules and the metabolism of xenobiotics. CYP2B4 can metabolize substituted amines, while CYP2E1 metabolizes various alcohols and halogenated alkenes.

In vitro: 4-phenyl-5-methyl-1,2,3-Thiadiazole (PMT) was found to be slightly more inhibitory to P450s 2E1 and 1A2 than its close analog, 4,5-diphenyl-1,2,3-thiadiazole (DPT). By contrast, 4-phenyl-5-hydrogen-1,2,3-Thiadiazole (PT), a weaker inhibitor than DPT and PMT with P450s 2E1 and 2B4, was comparable to PMT and more effective than DPT with P450 1A2. Moreover, PMT, DPT, as well as PT showed no inactivation of either P450 2E1 or 2B4, though they were fairly effective inhibitors, and the thiadiazole ring could be oxidized by the P450 system. Furthermore, the lack of inactivation of the P450 isoforms by PMT, DPT, and PT suggested that a transient reactive intermediate was not

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formed on oxidation of the thiadiazole ring. In addition, the 1,2,3-thiadiazole ring could be oxidized by the P450 system [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).

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