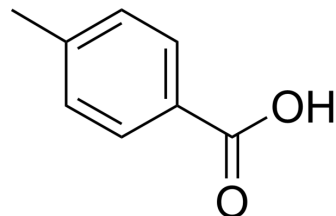


p-Toluic acid

Cat. No.:	HY-76547
CAS No.:	99-94-5
Molecular Formula:	C ₈ H ₈ O ₂
Molecular Weight:	136.15
Target:	Endogenous Metabolite
Pathway:	Metabolic Enzyme/Protease
Storage:	Store at room temperature 3 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro	DMSO : 100 mg/mL (734.48 mM; Need ultrasonic)					
	Preparing Stock Solutions	Solvent Concentration	Mass	1 mg	5 mg	10 mg
			1 mM	7.3448 mL	36.7242 mL	73.4484 mL
			5 mM	1.4690 mL	7.3448 mL	14.6897 mL
			10 mM	0.7345 mL	3.6724 mL	7.3448 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 (18.36 mM); Clear solution					
	2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (18.36 mM); Clear solution					
	3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (18.36 mM); Clear solution					

BIOLOGICAL ACTIVITY

Description	p-Toluic acid (4-Methylbenzoic acid), coumarin, is a substituted benzoic acid. p-Toluic acid is synthetic p-aminomethylbenzoic acid (PAMBA), intermediates such as p-toluonitrile. p-Toluic acid may have potential reproductive toxicity, press 1g/kg. Repeated administration of doses can produce a variety of adverse effects on the epididymis ^{[1][2]} .
IC ₅₀ & Target	Human Endogenous Metabolite
In Vivo	In reproductive/developmental studies, p-Toluic acid (1 g/kg; po, once daily for 28 days) decreases epididymal weight and increases the incidence of oligozoospermia/azoospermia in the cauda epididymis in rats ^[2] .

p-Toluic acid doesn't show any adverse effects on the animal's reproductive organs at doses of 0, 100, 300 or 1,000 mg/kg and doesn't affect the estrous cycle or mating performance. The NOEL for p-Toluic acid in male and female rats are considered to be 300 mg/kg^[2].

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

Animal Model:	Male and female rats ^[2]
Dosage:	0, 100, 300, 1,000 mg/kg
Administration:	po; once daily for 28 days
Result:	Resulted temporal salivation, a slight increase in food consumption and a moderate increase in blood aspartate aminotransferase (AST) activity under 1000 mg/kg dose. NOEL is considered to be 300 mg/kg for male and female rats.

CUSTOMER VALIDATION

- Laurea Magistrale in Biomedical Engineering, Politecnico di Milano. 2019 Jun.

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REFERENCES

- [1]. Pfennig T, et al. The formation of p-toluic acid from coumalic acid: a reaction network analysis[J]. Green Chemistry, 2017, 19(14): 3263-3271.
- [2]. Shirota M, et al. Screening of toxicological properties of 4-methylbenzoic acid by oral administration to rats. J Toxicol Sci. 2008 Oct;33(4):431-45.

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

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