Product Data Sheet

Product Name: N-Benzylacetamidine (hydrobromide)
Cat. No.: GC12677

Chemical Properties

Cas. No.	186545-76-6		
Chemical Name	N-(phenylmethyl)-ethanimidamide, monohydrobromide		
SMILES	CC(NCC1=CC=CC=C1)=N.Br		
Formula	$C_9H_{12}N_2 \cdot HBr$	M.Wt	229.1
Solubility	≤25mg/ml in ethanol;15mg/ml in DMSO;20mg/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

IC50: 0.20 μM: inhibits inducible nitric oxide synthases (iNOS).

IC50: 350 μM: blocks endothelial nitric oxide synthases (eNOS).

N-Benzylacetamidine is a potent and selective inhibitor of iNOS compared to eNOS. NOS is essential to the formation of nitric oxide (NO) via the NADPH- and O2-dependent oxidation of L-arginine, which plays a role in regulating many pathological and physiological processes, including smooth muscle relaxation and neurotransmission. INOS contributes to immune response and inflammation while eNOS plays a vital role in regulating vascular tone.

In vitro: N-Benzylacetamidine showed good iNOS and almost negligible eNOS inhibition in THP-1 cells, a human myelomonocytic leukemia cell line [1].

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In vivo: Up to now, in vivo study of N-Benzylacetamidine is still in the development stage.

Reference:

[1]. Maccallini, C., Patruno, A., Besker, N., Ali, J., Ammazzalorso, A., & De Filippis, B. et al. Synthesis, Biological Evaluation, and Docking Studies of N-Substituted Acetamidines as Selective Inhibitors of Inducible Nitric Oxide Synthase. Journal of Medicinal Chemistry. 2009; 52(5): 1481-1485.

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