Product Data Sheet

Product Name:	S-ethyl N-[4-(trifluoromethyl)phenyl] Isothiourea (hydrochloride)
Cat. No.:	GC10851

Chemical Properties

Cas. No.	163490-78-6		
Chemical Name	ethyl[4-(trifluoromethyl)phenyl] carbamimidothioate, hydrochloride		
SMILES	CCS/C(N([H])C1=CC=C(C(F)(F)F)C=C1)=N\[H].Cl		
Formula	$C_{10}H_{11}F_3N_2S \cdot HCl$	M.Wt	284.7
Solubility	≤34mg/ml in ethanol;34mg/ml in DMSO;34mg/ml in dimethyl formamide;50mg/ml in Water	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

S-ethyl N-[4-(trifluoromethyl)phenyl] Isothiourea (hydrochloride) is a selective and competitive nNOS inhibitor with Ki value of 0.32 μM for the purified human enzyme [1].

Nitric oxide (NO) is an endogenously produced inorganic free radical gas which has been implicated in blood pressure homeostasis, platelet aggregation, neurotransmission, and immunological defense mechanisms. NO is synthesized by three isoforms of nitric oxide synthase (NOS): nNOS, eNOS and iNOS [1].

S-ethyl N-[4-(trifluoromethyl)phenyl] Isothiourea (hydrochloride) (EPIT) is a selective and competitive nNOS inhibitor. S-ethyl N-[4-(trifluoromethyl)phenyl] Isothiourea inhibited human nNOS, eNOS and iNOS with Ki values of 0.32 μM, 9.4 μM and 37 μM, respectively. EPIT exhibited 115-fold and 29-fold selectivity for nNOS compared to iNOS and eNOS, respectively [1].

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

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In mice, EPIT administered intravenously at 25 mg/kg readily penetrated the blood-brain barrier, immediately reaching concentrations in the brain equal to the plasma concentration. In rat brain slices, EPIT failed to inhibit nNOS activity, possibly due to reduced intracellular uptake [1].

Reference:

[1]. Shearer BG, Lee S, Oplinger JA, et al. Substituted N-phenylisothioureas: potent inhibitors of human nitric oxide synthase with neuronal isoform selectivity. J Med Chem. 1997 Jun 6;40(12):1901-5.

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