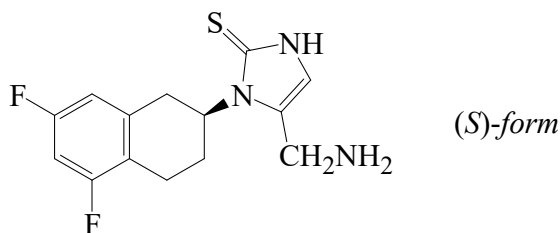




>>Entry Name: Nepicastat, INN

Synonym(s): 5-(Aminomethyl)-1-(5,7-difluoro-1,2,3,4-tetrahydro-2-naphthalenyl)-1,3-dihydro-2*H*-imidazole-2-thione, 9Cl. 2-(5-Aminomethyl-1,3-dihydro-2-thioxoimidazol-3-yl)-5,7-difluoro-1,2,3,4-tetrahydronaphthalene



CAS Registry Number: 170151-25-4

Related CAS Registry Numbers(s): 173997-06-3 195881-94-8

Molecular Formula: C₁₄H₁₅F₂N₃S

Molecular Weight: 295.355

Accurate Mass: 295.095473

Percentage Composition: C 56.93%; H 5.12%; F 12.86%; N 14.23%; S 10.86%

Biological Use/Importance: Dopamine β-hydroxylase inhibitor. Inhibits noradrenaline synthesis. Potential agent for treating cardiovascular disorders associated with overactivation of sympathetic nervous system. Antihypertensive agent

Melting Point: Mp 172-178°

>>Variant: (S)-form

Synonym(s): RS 25560-197

CAS Registry Number: 173997-05-2

Molecular Formula: C₁₄H₁₅F₂N₃S

Molecular Weight: 295.355

Accurate Mass: 295.095473

Percentage Composition: C 56.93%; H 5.12%; F 12.86%; N 14.23%; S 10.86%

Other Data: Pharmacol. active isomer

>>Derivative: Hydrochloride

Synonym(s): Nepicastat hydrochloride, USAN

CAS Registry Number: 170151-24-3

Physical Description: Solid

Melting Point: Mp 245°

Hazard & Toxicity: LD (mus, orl) 1000 mg/kg. Lacks mutagenic props.

References:

Pat. Coop. Treaty (WIPO), 1995, Syntex, 95 29 165; CA, **124**, 176116k, (synth, pharmacol)
Stanley, W.C. et al., Br. J. Pharmacol., 1997, **121**, 1803-1809, (pharmacol)