

Product Data Sheet

Product Name: CAY10729 (trifluoroacetate salt) (technical grade)

Cat. No.: GC45402

Chemical Properties

Cas. No.

SMILES O=C(N[C@@H](CCCNC(CCl)=N)C1=NN(C(C)(C)C)N=N1)C2=CC=CC=C2C(O)=O.FC(F)(C(O)=O)F

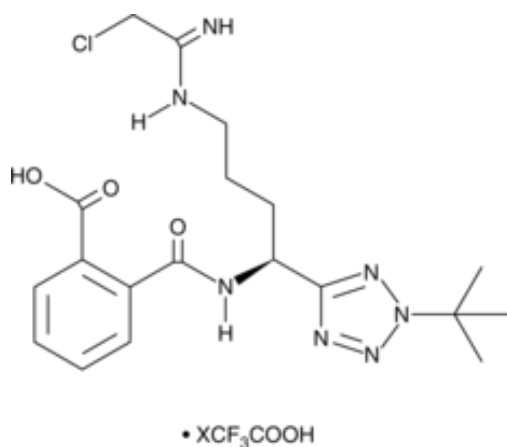
Formula C₁₉H₂₆ClN₇O₃.XCF₃COOH M.Wt 435.9

Solubility Methyl Acetate: Soluble 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



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

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Address: 10292 Central Ave. #205, Montclair, CA, USA

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Background

CAY10729 is a tetrazole derivative of the protein arginine deiminase (PAD) inhibitor Cl-amidine that selectively inhibits PAD1 over PAD2, PAD3, and PAD4 ($k_{\text{inact}}/K_i = 162,200, 60,000, 17,500,$ and $25,400 \text{ M}^{-1}\text{min}^{-1}$ for PAD1-4, respectively).¹

References

1. Subramanian, V., Knight, J.S., Parelkar, S., et al. Design, synthesis, and biological evaluation of tetrazole analogs of cl-amidine as protein arginine deiminase inhibitors. *Journal of Medicinal Chemistry* 58(3), 1337-1344 (2015).

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