
Product Data Sheet

Product Name: IDH1 Inhibitor 3

Cat. No.: GC36293

Chemical Properties

Cas. No. 2171081-24-4

SMILES O=C([C@@H](CC1)N(C2=NC=CC(C#N)=C2)C1=O)N([C@@]3(C(NC4CC(F)(F)C4)=O)CCC5=C3C=CC=C5)C6=CC(F)=CC(F)=C6Formula C₃₁H₂₅F₄N₅O₃ M.Wt 591.56

Solubility Soluble in DMSO 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 **Background**

IDH1 Inhibitor 3 (compound 6f) is a mutant isocitric dehydrogenase 1 (IDH1) inhibitor, with an IC₅₀ of 45 nM for IDH1R132H[1]. IC₅₀: 45 nM (IDH1R132H)[1].

[1]. Qiangang Zheng, et al. Discovery and structure-activity-relationship study of novel conformationally restricted indane analogues for mutant isocitric dehydrogenase 1 (IDH1) inhibitors. *Bioorganic & Medicinal Chemistry Letters* 27 (2017) 5262-5266.

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

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