
Product Data Sheet

Product Name: mPGES1-IN-3

Cat. No.: GC36649

Chemical Properties

Cas. No. 1469976-70-2

SMILES O=C(NC1=CC(F)=CC(C(F)(F)F)=C1)C2=C(OCCO3)C3=C(N(C)C(NC4=C(Cl)C=CC=C4F)=N5)C5=C2Formula $C_{24}H_{16}ClF_5N_4O_3$ M.Wt 538.85

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**

mPGES1-IN-3 (Compound 17d) is a potent and selective microsomal prostaglandin E2 synthase-1 (mPGES-1) inhibitor, which exhibits excellent mPGES-1 enzyme (IC₅₀: 8 nM), cell (A549 IC₅₀: 16.24 nM) and human whole blood potency (IC₅₀: 249.9 nM)[1]. IC₅₀: 8 nM (mPGES-1)[1]

[1]. Muthukaman N, et al. Discovery of 2-((2-chloro-6-fluorophenyl)amino)-N-(3-fluoro-5-(trifluoromethyl)phenyl)-1-methyl-7,8-dihydro-1H-[1,4]dioxino[2',3':3,4]benzo[1,2-d]imidazole-5-carboxamide as potent, selective and efficacious microsomal prostaglandin E2 synthase-1 (mPGES-1) inhibitor. *Bioorg Med Chem Lett.* 2016 Dec 15;26(24):5977-5984.

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

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