



Product Information

Isocitrate dehydrogenase (IDH) inhibitor, AGI-6780, Purity $\geq 98\%$

Cat. No.: X24-09-YM319

Size: 5 mg; 10 mg; 25 mg; 50 mg

MDL: MFCD26097285

CAS Number: 1432660-47-3

Compound CID: 71299339

Synonym: 1432660-47-3; AGI6780;

N

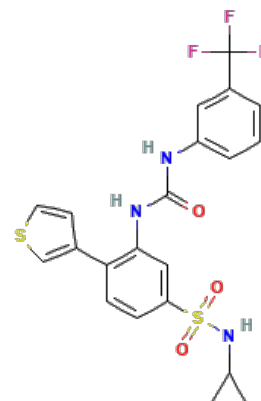
-Cyclopropyl-4-(thiophen-3-yl)-3-(3-(3-(trifluoromethyl)phenyl)ureido)benzenesulfonam

ide; AGI 6780;

1-[5-(Cyclopropylsulfamoyl)-2-thiophen-3-ylphenyl]-3-[3-(trifluoromethyl)phenyl]urea;

Isocitrate dehydrogenase (IDH) inhibitor

This product is for research use only and is not intended for diagnostic use.



Product Information

Description	AGI-6780, soluble in DMSO and ethanol and insoluble in water, is an effective metabolism inhibitor, that has the ability to prevent the pathway of cell metabolism by inhibiting isocitrate dehydrogenase (IDH). The molecular weight of the compound is 481.5, and its molecular formula is C ₂₁ H ₁₈ F ₃ N ₃ O ₃ S. It targets the IDH2 R140Q mutant.
Molecular Weight	481.5
Molecular Formula	C ₂₁ H ₁₈ F ₃ N ₃ O ₃ S
Targets	IDH2 R140Q mutant
IUPAC Name	1-[5-(Cyclopropylsulfamoyl)-2-thiophen-3-ylphenyl]-3-[3-(trifluoromethyl)phenyl]urea
InChI	InChI=1S/C21H18F3N3O3S2/c22-21(23,24)14-2-1-3-16(10-14)25-20(28)26-19-11-17(32(29,30)27-15-4-5-15)6-7-18(19)13-8-9-31-12-13/h1-3,6-12,15,27H,4-5H2,(H2,25,26,28)
InChI Key	CCAWRGNYALGPQH-UHFFFAOYSA-N
Canonical SMILES	C1CC1NS(=O)(=O)C2=CC(=C(C=C2)C3=CSC(=C3)NC(=O)NC4=CC=CC(=C4)C(F)(F)F
Isomeric SMILES	C1CC(=O)N([C@@H]1C(=O)N(C2=CC(=CN=C2)F)C(C3=CC=CC=C3Cl)C(=O)NC4CC(C4)(F)F)C5=NC=CC(=C5)C#N
Form	Lyophilized powder
Purity	$\geq 98\%$



Impurities	Free from inappropriate visible particulates, foreign matter, discoloration, or other defects.
Solubility	<i>In vitro</i> : DMSO: 87 mg/mL (180.68 mM); Water: insoluble; Ethanol: 87 mg/mL (180.68 mM)
Identity	Confirmed by NMR/HPLC/MS.
Stability	In its lyophilized form, the chemical remains stable for 36 months.
Quality Level	Research grade
Applications	AGI-6780 can be studied extensively for its potential therapeutic applications in the treatment of cancers associated with IDH1 mutations.
Storage	Store at -20°C, and keep desiccated.