



IKK-16 (IKK Inhibitor VII)

Cat. No.:	OB0225WX-2533
Appearance:	Solid
Purity:	≥99%
Identity:	Confirmed by NMR, and HPLC.
Size:	10 mg; 50 mg; 1 g

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

Product Overview

Description	IKK-16 is a multi-IKK inhibitor targeting IKK-2, the IKK complex, and IKK-1 (IC ₅₀ : 40 nM, 70 nM, and 200 nM) that also suppresses LRRK2 kinase activity.
Synonym	873225-46-8; IKK Inhibitor VII; IKK 16; IKK-16; IKK-16 (IKK Inhibitor VII); IKK1 6; IKK-16 (free base); IKK Inhibitor; (4-((4-(Benzo[b]thiophen-2-yl)pyrimidin-2-yl)amino)phenyl)(4-(pyrrolidin-1-yl)piperidin-1-yl)methanone; 873225-46-8 (free base); [4-[[4-(1-benzothiophen-2-yl)pyrimidin-2-yl]amino]phenyl]-(4-pyrrolidin-1-yl)piperidin-1-yl)methanone; [4-[(4-Benzo[b]thien-2-yl-2-pyrimidinyl)amino]phenyl][4-(1-pyrrolidinyl)-1-piperidinyl]-Methanone; (4-{[4-(1-benzothiophen-2-yl)pyrimidin-2-yl]amino}phenyl)[4-(pyrrolidin-1-yl)piperidin-1-yl]methanone; 4-(1-benzothiophen-2-yl)-N-{4-[4-(pyrrolidin-1-yl)piperidine-1-carbonyl]phenyl}pyrimidin-2-amine; K00596a; MFCD23704180
CAS No.	873225-46-8
Compound CID	9549298
Formula	C ₂₈ H ₂₉ N ₅ OS
Formula Weight	483.63

Specification

IUPAC Name	[4-[[4-(1-Benzothiophen-2-yl)pyrimidin-2-yl]amino]phenyl]-(4-pyrrolidin-1-yl)piperidin-1-yl)methanone
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InChI	InChI=1S/C28H29N5OS/c34-27(33-17-12-23(13-18-33)32-15-3-4-16-32)20-7-9-22(10-8-20)30-28-29-14-11-24(31-28)26-19-21-5-1-2-6-25(21)35-26/h1-2,5-11,14,19,23H,3-4,12-13,15-18H2,(H,29,30,31)
InChI Key	BWZJBXAPRCVCKQ-UHFFFAOYSA-N
SMILES string	C1CCN(C1)C2CCN(CC2)C(=O)C3=CC=C(C=C3)NC4=NC=CC(=N4)C5=CC6=CC=CC=C6S5
Stability	3 years in powder form.
Storage	Storage at -20°C.
Applications	IKK-16 is employed in signal transduction research as a selective IKK complex inhibitor to investigate the disruption of the NF-kappaB signaling axis and its role in chronic inflammatory responses.

Library Information

Target	IκB/IKK; LRRK2
Receptor	IKK; LRRK2
Pathways	NF-κB
Plate Number	L6700-05
Empty Location	a1-h1; a12-h12
Container	96-well plate
Formulation	10mM DMSO
DMSO Max Solubility	97 mg/mL; 200.57 mM
ALogP	5.208
HBA_Count	3
HBD_Count	1
Rotatable Bond	5