



AEE788 (NVP-AEE788)

Cat. No.:	OB0225WX-2419
Appearance:	Solid
Purity:	≥99%
Identity:	Confirmed by NMR, and HPLC.
Size:	5 mg; 10 mg; 25 mg; 50 mg

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

Product Overview

Description	AEE788 (NVP-AEE788) is a potent dual inhibitor of EGFR (IC ₅₀ : 2 nM) and HER2/Erb B2 (IC ₅₀ : 6 nM), while showing minimal activity against Ins-R or IGF-1R.
Synonym	497839-62-0; AEE788; AEE-788; AEE 788; NVP-AEE788; (R)-6-(4-((4-Ethylpiperazin-1-yl)methyl)phenyl)-N-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-amine; NVP-AEE-788; 6-{4-[(4-Ethylpiperazin-1-yl)methyl]phenyl}-N-[(1R)-1-Phenylethyl]-7h-Pyrrolo[2,3-D]pyrimidin-4-Amine; 6-[4-[(4-ethylpiperazin-1-yl)methyl]phenyl]-N-[(1R)-1-phenylethyl]-7H-pyrrolo[2,3-d]pyrimidin-4-amine; 7H-pyrrolo(2,3-d)pyrimidin-4-amine, 6-(4-((4-ethyl-1-piperazinyl)methyl)phenyl)-N-((1R)-1-phenylethyl)-; (R)-6-(4-((4-ethylpiperazin-1-yl)methyl)phenyl)-N-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-amine.; 5-[(2-Chlorophenyl)methyl]-4,5,6,7-tetrahydro-5-methylthieno[3,2-c]pyridinium iodide; AEE; MFCD11100351; 6-[4-[(4-Ethyl-1-piperazinyl)methyl]phenyl]-N-[(1R)-1-phenylethyl]-7H-pyrrolo[2,3-d]pyrimidin-4-amine; [6-[4-[(4-ethyl piperazin-1-yl)methyl]phenyl]-7h-pyrrolo[2,3-d]pyrimidin-4-yl]-((r)-1-phenylethyl)amine; 1H-Pyrrolo(2,3-d)pyrimidin-4-amine, 6-(4-((4-ethyl-1-piperazinyl)methyl)phenyl)-N-((1R)-1-phenylethyl)-; 6-[4-[(4-ethylpiperazin-1-yl)methyl]phenyl]-N-[(1R)-1-phenylethyl]-7H-pyrrolo[3,2-e]pyrimidin-4-amine; 6-{4-[(4-ethyl-1-piperazinyl)methyl]phenyl}-N-[(1R)-1-phenylethyl]-1H-pyrrolo[2,3-d]pyrimidin-4-amine
CAS No.	497839-62-0
Compound CID	10297043



Formula $C_{27}H_{32}N_6$

Formula Weight 440.58

Specification

IUPAC Name 6-[4-[(4-Ethylpiperazin-1-yl)methyl]phenyl]-N-[(1R)-1-phenylethyl]-7H-pyrrolo[2,3-d]pyrimidin-4-amine

InChI InChI=1S/C27H32N6/c1-3-32-13-15-33(16-14-32)18-21-9-11-23(12-10-21)25-17-24-26(28-19-29-27(24)31-25)30-20(2)22-7-5-4-6-8-22/h4-12,17,19-20H,3,13-16,18H2,1-2H3,(H2,28,29,30,31)/t20-m/s1

InChI Key OONFNUWBHFSNBT-HXUWFJFHSA-N

SMILES string CCN1CCN(CC1)CC2=CC=C(C=C2)C3=CC4=C(N3)N=CN=C4N[C@H](C)C5=CC=CC=C5

Stability 3 years in powder form.

Storage Storage at -20°C.

Applications AEE788 (NVP-AEE788) is utilized in signal transduction research as a multi-targeted inhibitor of EGFR and VEGFR family kinases to investigate the simultaneous blockade of tumor growth and vascularization.

Library Information

Target EGFR; HER2; VEGFR

Receptor EGFR; HER2; VEGFR

Pathways Protein tyrosine kinase

Plate Number L6700-02

Empty Location a1-h1; a12-h12

Container 96-well plate

Formulation 10mM DMSO

DMSO Max Solubility 88 mg/mL; 199.74 mM

ALogP 5.042

HBA_Count 2

HBD_Count 2

Rotatable Bond 7