Typical Product Specifications & Properties

NNC 0640

CAS Number: : 307986-98-7

Specifications	Limits
Chemical Structure	chemicalStructure-nnc-0640
Molecular Formula	C29H31N7O4S
Molecular weight	
Canonicalized Compound	1
Compound Complexity	970
Hydrogen Bond Acceptor Count	7
Hydrogen Bond Donor Count	3
Rotatable Bond Count	8
Allowed IUPAC Name	4-[[4-cyclohexyl-N-[(3-methylsulfonylphenyl)carbamoyl]anilino]methyl]-N-(2H-tetrazol-5-yl)benzamide
CAS-like Style IUPAC Name	4-[(4-cyclohexyl-N-[(3-methylsulfonylanilino)-oxomethyl]anilino)methyl]-N-(2H-tetrazol-5-yl)benzamide
Markup IUPAC Name	4-[[4-cyclohexyl-<I>N</I>-[(3-methylsulfonylphenyl)carbamoyl]anilino]methyl]-<I>N</I>-(2<I>H</I>-tetrazol-5-yl)benzamide
Preferred IUPAC Name	4-[[4-cyclohexyl-N-[(3-methylsulfonylphenyl)carbamoyl]anilino]methyl]-N-(2H-tetrazol-5-yl)benzamide

Specifications	Limits
Systematic IUPAC Name	4-[[(4-cyclohexylphenyl)-[(3-methylsulfonylphenyl)carbamoyl] yl)benzamide
Traditional IUPAC Name	4-[[4-cyclohexyl-N-[(3-mesylphenyl)carbamoyl]anilino]methyl]
Standard InChI	InChI=1S/C29H31N7O4S/c1-41(39,40)26-9-5-8-24(18-26)30-29(3 21)19-20-10-12-23(13-11-20)27(37)31-28-32-34-35-33-28/h5,8-18, (H2,31,32,33,34,35,37)
Standard InChIKey	PPTKULJUDJWTSA-UHFFFAOYSA-N
XLogP3-AA Log P	4.7
Exact Mass	573.21582367
Molecular Weight	573.7

Specifications	Limits
Canonical SMILES	CS(=O) (=O)C1=CC=CC(=C1)NC(=O)N(CC2=CC=C(C=C2)C(=O)NC3
Isomeric SMILES	CS(=O) (=O)C1=CC=CC(=C1)NC(=O)N(CC2=CC=C(C=C2)C(=O)NC3
Polar Surface Area	158

Aled Topological	156
Monolsotopic Weight	573.21582367