Typical Product Specifications & Properties

N-(1,3-benzodioxol-5-ylmethyl)-4-([1]benzofuro[3,2-d]pyrimidin-4-yl)piperazine-1-carbothioamide

CAS Number: : 850879-09-3

Specifications	Limits
Molecular Formula	C23H21N5O3S
Molecular weight	
Canonicalized Compound	1
Compound Complexity	678
Hydrogen Bond Acceptor Count	7
Hydrogen Bond Donor Count	1
Rotatable Bond Count	3
Allowed IUPAC Name	N-(1,3-benzodioxol-5-ylmethyl)-4-(benzofuro[3,2-d]pyrimidin-4-yl)piperazine-1-carbothioamide
CAS-like Style IUPAC Name	N-(1,3-benzodioxol-5-ylmethyl)-4-(4-benzofuro[3,2-d]pyrimidinyl)-1-piperazinecarbothioamide
Markup IUPAC Name	<I>N</I>-(1,3-benzodioxol-5-ylmethyl)-4-([1]benzofuro[3,2-d]pyrimidin-4-yl)piperazine-1-carbothioamide
Preferred IUPAC Name	N-(1,3-benzodioxol-5-ylmethyl)-4-([1]benzofuro[3,2-d]pyrimidin-4-yl)piperazine-1-carbothioamide
Systematic IUPAC Name	N-(1,3-benzodioxol-5-ylmethyl)-4-([1]benzofuro[3,2-d]pyrimidin-4-yl)piperazine-1-carbothioamide

Specifications	Limits
Traditional IUPAC Name	4-(benzofuro[3,2-d]pyrimidin-4-yl)-N-piperonyl-piperazine-1-carb
Standard InChI	InChI=1S/C23H21N5O3S/c32-23(24-12-15-5-6-18-19(11-15)30-14 10-28)22-21-20(25-13-26-22)16-3-1-2-4-17(16)31-21/h1-6,11,13H, (H,24,32)
Standard InChIKey	FOFDIMHVKGYHRU-UHFFFAOYSA-N
XLogP3-AA Log P	3.5
Exact Mass	447.13651072
Molecular Weight	447.5
Canonical SMILES	C1CN(CCN1C2=NC=NC3=C2OC4=CC=CC=C43)C(=S)NCC5=

Specifications	Limits
Isomeric SMILES	C1CN(CCN1C2=NC=NC3=C2OC4=CC=CC=C43)C(=S)NCC5=
Polar Surface Area	108
Topological	

Monoisotopic Weight	447.13651072
Chemical Structure