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## 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            | <l>N</l>-(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        |

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| 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      | FOFDIMHVKG YHRU-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=

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Polar Surface Area

108

Topological

Molecular

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Monoisotopic  
Weight

Chemical  
Structure

447.13651072

chemicalStructure-n-1-3-benzodioxol-5-ylmethyl-4-1-benzofur  
piperazine-1-carbothioamide



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