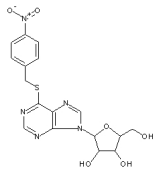

Formula: C17H17N5O6S

MW: 419.42

CAS: 38048-32-7

MDL NUMBER: MFCD00323601

Smiles: C(C1OC(n2c3c(c(SCc4ccc(cc4)[N+]([O-])=O)ncn3)nc2)C(C1O)O)O

Neurotransmitters > Adenosines/P2 Nucleotide Receptors (Purinergics)

ACCEPTORS: 6

DONORS: 3

ROTATION BONDS: 7

N+O: 11

Chiral Centers: 4

LogP: -0.43

LogS: -3.5

LIPINSKI: 4

Synonyms:
6-[(4-NITROBENZYL)THIO]-9-BETA-D-RIBOFURANOSYLPURINE;S-(P-NITROBENZYL)-6-THIOINOSINE;S-(4-NITROBENZYL)-6-THIOINOSINE;NBMPR;NBTI;4-nitrobenzylthioinosine;6-(((4-nitrophenyl)methyl)thio)-9-beta-d-ribofuranosyl-9h-purin;6-(((4-nitrophenyl)methyl)thio)-9-beta-d-ribofuranosyl-9h-purine

CAS:38048-32-7

MF:C17H17N5O6S

MW:419.41

EINECS:253-753-4

Product Categories:Bases & Related Reagents;Heterocycles;Inhibitors;Nucleotides;Sulfur & Selenium Compounds S-(4-NITROBENZYL)-6-THIOINOSINE

Chemical Properties: mp 187-190 C(lit.) storage temp. 2-8C solubility 0.1 M HCl: slightly soluble form solid color white

CAS DataBase Reference: 38048-32-7(

CAS DataBase Reference:)

Safety Information: Safety Statements 24/25 WGK Germany 3 RTECS UO9025000 S-(4-NITROBENZYL)-6-THIOINOSINE

Usage And Synthesis:

Chemical Properties: Off-White Solid UsageIt is a prototype inhibitor of the human equilibrative nucleoside transporter (hENT1), and is a high affinity ligand with a Kd of 0.1-1.0 nM. Nucleoside transporter inhibitors have potential therapeutic applications as anticancer, antiviral, cardio Biological ActivityEquilibrative nucleoside transporter 1 (ENT1) inhibitor (K i values are 0.4 and 2800 nM for hENT1 and hENT2 respectively). S-(4-NITROBENZYL)-6-THIOINOSINE