



Product Information

2-Chloro-*N*-[(3-iodophenyl)methyl]-2', 3'-*O*-(1-methylethylidene) adenosine

Cat. No.: X24-03-LY005

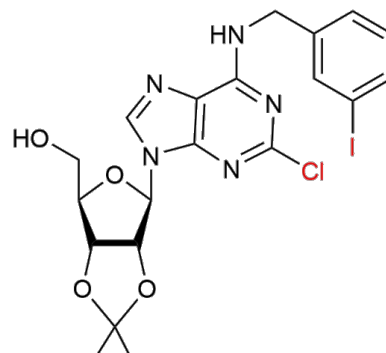
Size: 5 g; 10 g; 25 g; 100 g

MDL: MFCD30475782

CAS Number: 1000980-71-1

PubChem CID: 122173512

Synonym: 1000980-71-1; 2-Chloro-*N*-(3-iodobenzyl)-2', 3'-*O*-isopropylideneadenosine; (3*aR*, 4*R*, 6*R*, 6*aR*)-4-[2-Chloro-6-[(3-iodophenyl)methylamino]purin-9-yl]-2, 2-dimethyl-3*a*, 4, 6, 6*a*-tetrahydrofuro[3, 4-*d*][1, 3]dioxol-6-yl)methanol; [(3*aR*, 4*R*, 6*R*, 6*aR*)-6-(2-Chloro-6-[(3-iodophenyl)methyl]amino}-9*H*-purin-9-yl)-2, 2-dimethyl-tetrahydro-2*H*-furo[3, 4-*d*][1, 3]dioxol-4-yl)methanol



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

Product Information

Description	2-Chloro- <i>N</i> -[(3-iodophenyl)methyl]-2', 3'- <i>O</i> -(1-methylethylidene) adenosine is an adenosine derivative containing chlorine and iodine substituents.
Molecular Weight	557.77
Molecular Formula	C ₂₀ H ₂₁ ClINN ₅ O ₄
IUPAC Name	[(3 <i>aR</i> ', 4 <i>R</i> , 6 <i>R</i> , 6 <i>aR</i> ')-4-[2-Chloro-6-[(3-iodophenyl)methylamino]purin-9-yl]-2, 2-dimethyl-3 <i>a</i> , 4, 6, 6 <i>a</i> -tetrahydrofuro[3, 4- <i>d</i>][1, 3]dioxol-6-yl)methanol
InChI	InChI=1S/C20H21ClIN5O4/c1-20(2)30-14-12(8-28)29-18(15(14)31-20)27-9-24-13-16(25-19(21)26-17(13)27)23-7-10-4-3-5-11(22)6-10/h3-6, 9, 12, 14-15, 18, 28H, 7-8H2, 1-2H3, (H, 23, 25, 26)/t12-, 14-, 15-, 18-/m1/s1
InChI Key	WCKHUABYZBGHID-SCFUHWHPSA-N
Canonical SMILES	CC1(OC2C(OC(C2O1)N3C=NC4=C(N=C(N=C43)Cl)NCC5=CC(=CC=C5)I)CO)C
Isomeric SMILES	CC1(O[C@@H]2[C@H](O[C@H]([C@@H]2O1)N3C=NC4=C(N=C(N=C43)Cl)NCC5=CC(=CC=C5)I)CO)C
Form	White to off-white solid
Purity	≥95%
Applications	2-Chloro- <i>N</i> -[(3-iodophenyl)methyl]-2', 3'- <i>O</i> -(1-methylethylidene) adenosine has potential applications in the field of medicine.



Storage

Store at -20°C.

Safety Information

Personal Protective Equipment	Gloves, eyeshields, N95 mask
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Hazard Statements	H302-H315-H319-H335
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