



Formula: C₃₀H₂₄N₄O₁₀

MW: 600.54

CAS: 15351-13-0

MDL NUMBER: MFCD09788227

IUPAC: (2S,4S,5S,3R)-2,5-bis(3-pyridylcarbonyloxymethyl)-2-hydroxy-4-(3-pyridylcarbonyloxymethyl)oxolan-3-yl pyridine-3-carboxylate

Smiles:

c1(cccnc1)C(OC[C@@H]1O[C](O)([C@@H]([C@H]1OC(=O)c1ccnc1)OC(c1ccnc1)=O)COC(=O)c1ccnc1)=O

THERAPEUTIC CATEGORY: Vasodilator (Peripheral)

ACCEPTORS: 10

DONORS: 1

ROTATION BONDS: 11

N+O: 14

Chiral Centers: 4

LogP: 0.22

LogS: -4.66

LIPINSKI: 3

Synonyms: NICOFURANOSE;BETA-D-FRUCTOFURANOSE
TETRANICOTINATE;1,3,4,6-Tetrakis-O-(3-pyridinylcarbonyl)hex-2-ulofuranose;beta-D-Fructofu
ranose, 1,3,4,6-tetra-3-pyridinecarboxylate;Bradilan;D-Fructofuranose
1,3,4,6-tetranicotinate;Vasperdil;