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Typical Product Specifications & Properties

1-[2-Chloro-6-[[[3-Iodophenyl)Methyl]Amino]-9H-Purin-9-Yl]-1-Deoxy-N-Methyl-Beta-D-Ribofuranuronamid

CAS Number: : 163042-96-4

Specifications	Limits
Molecular weight	544.73
SMILES	<chem>CNC(=O)[C@@H]1[C@H]([C@H]([C@@H](O1)n2cnc3c2nc(nc3NCC4CCCC(C4)I)Cl)O)O</chem>
InChI	IPSYPUKKXMNCNQ-PFHKOEEOSA-N
InChIKey	1S/C18H18ClIN6O4/c1-21-16(29)13-11(27)12(28)17(30-13)26-7-23-10-14(24-18(19)25-15(10)26)22-6-8-3-2-4-9(20)5-8/h2-5,7,11-13,17,27-28H,6H2,1H3,(H,21,29)(H,22,24,25)/t11-,12+,13-,17+/m0/s1



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