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Typical Product Specifications & Properties

7-Deazaadenosine; Antibiotic XK 101-1; N7-Deazaadenosine; NSC 56408; Sparsomycin A; Tubercidine; U 10

CAS Number: : 69-33-0

Specifications	Limits
Molecular weight	266.25
EINECS	200-703-4
SMILES	<chem>n1(c2c(c(ncn2)N)cc1)[C@@H]1O[C@H](CO)[C@H]([C@H]1O)O</chem>
InChI	HDZZVAMISRMYHH-KCGFPETGSA-N
InChIKey	1S/C11H14N4O4/c12-9-5-1-2-15(10(5)14-4-13-9)11-8(18)7(17)6(3-16)19-11/h1-2,4,6-8,11,16-18H,3H2,(H2,12,13,14)/t6-,7-,8-,11-/m1/s1
Henry's Law Constant	2.69E-22 atm-m ³ /mole
Water solubility	3000 mg/L
Atmospheric OH Rate Constant	2.38E-10 cm ³ /molecule-sec
Vapor Pressure	4.27E-13 mm Hg
log P (octanol-water)	-0.8



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