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Typical Product Specifications & Properties

Tetrodotoxin

CAS Number : 4368-28-9

Specifications	Limits
Molecular weight	319.27
EINECS	224-458-8
SMILES	<chem>NC1=N[C@H](O)[C@H]2[C@H]3O[C@]4(O)O[C@@H]([C@H](O)[C@@]2(N1)[C@@H]4O)[C@]3(O)CO</chem>
InChI	CFMYXEVWODSLAX-QYIGHCJRSA-N
InChIKey	1S/C11H17N3O8/c12-8-13-6(17)2-4-9(19,1-15)5-3(16)10(2,14-8)7(18)11(20,21-4)22-5/h2-7,15-20H,1H2,(H3,12,13,14)/t2-,3+,4-,5+,6-,7+,9+,10-,11+/m1/s1
log P (octanol-water)	-6.210
Atmospheric OH Rate Constant	3.71E-10 cm ³ /molecule-sec
pKa Dissociation Constant	8.76
Storage Temperature	2-8°C
Form	powder
Merck	13,9318
Solubility	H2O: stable at pH 4-5 if stored frozen soluble



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Specifications	Limits
Color	white



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