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Typical Product Specifications & Properties

Dinophysistoxin-1

CAS Number: : 81720-10-7

Specifications	Limits
Molecular weight	819.03
SMILES	<chem>C1CC[C@@H]([C@@]2(O1)O[C@@H]([C@@H](C[C@@H]([C@@H]1C(=C)[C@@H](O)[C@@H]3[C@@H](O1)CC[C@@]1(CC[C@@H](\C=C\ [C@@H]([C@@H]4CC(=C[C@@]5(O4)[C@@H](O)CC[C@@H](C[C@@](C(O)=O)(O)C)O5)C)C)O1)O3)O)C)[C@@H](CC2)C)C</chem>
InChI	CLBIEZ BAENPDFY-Z HACJKMWSA-N
InChIKey	1S/C45H70O13/c1-25-21-35(56-45(23-25)36(47)13-12-32(55-45)24-42(7,51)41(49)50)26(2)10-11-31-15-17-43(54-31)18-16-34-40(57-43)37(48)30(6)39(53-34)33(46)22-28(4)38-27(3)14-19-44(58-38)29(5)9-8-20-52-44/h10-11,23,26-29,31-40,46-48,51H,6,8-9,12-22,24H2,1-
Molecular weight	255.35
EINECS	200-396-7
SMILES	<chem>C(c1ccccc1)(c1ccccc1)OCCN(C)C</chem>
InChI	1S/C17H21NO/c1-18(2)13-14-19-17(15-9-5-3-6-10-15)16-11-7-4-8-12-16/h3-12,17H,13-14H2,1-2H3
InChIKey	ZZVUWRFHKOJYTH-UHFFFAOYSA-N
Henry's Law Constant	3.70E-09 atm-m ³ /mole
Vapor Pressure	3.70E-05 mm Hg
Melting Point	168 ° C



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Specifications	Limits
Atmospheric OH Rate Constant	1.27E-10 cm ³ /molecule-sec
pKa Dissociation Constant	8.98
log P (octanol-water)	3.27
Water solubility	3060 mg/L
Melting Point	167-172°C



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