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Typical Product Specifications & Properties

Veratridine

CAS Number: : 71-62-5

Specifications	Limits
Molecular weight	673.79
EINECS	200-758-4
SMILES	<chem>C1[C@@]23[C@H]([C@@]4(C[C@H](O)[C@@]5([C@H]([C@@]14O)C[N@@]1C[C@@H](C)CC[C@H]1[C@@]5(C)O)O)CC[C@H]1[C@@]2(CC[C@@]([C@@]1(O3)O)OC(c1cc(c(OC)cc1)OC)=O)C</chem>
InChI	FVECELJHCSPHKY-YFUMOZOISA-N
InChIKey	1S/C36H51NO11/c1-19-6-11-26-31(3,40)35(43)25(17-37(26)16-19)33(42)18-34-24(32(33,41)15-27(35)38)10-9-23-30(34,2)13-12-28(36(23,44)48-34)47-29(39)20-7-8-21(45-4)22(14-20)46-5/h7-8,14,19,23-28,38,40-44H,6,9-13,15-18H2,1-5H3/t19-,23-,24-,25-,26-,27-,28-,
log P (octanol-water)	3.760
Atmospheric OH Rate Constant	1.60E-10 cm ³ /molecule-sec
pKa Dissociation Constant	9.54
Melting Point	180 ° C

