

Typical Product Specifications & Properties

Thymidine-8-Methoxypsoralen Tetramethylethylene Diadduct

CAS Number: : 94591-68-1

Specifications	Limits
SMILES	<chem>O1[C@@H]2[C@@H]3[N@@]([C@H]4O[C@@H]([C@H](C4)O)CO)C(NC(=O)[C@@]3([C@@H]2c2c1c(c1c(c2)[C@@H]2[C@@H](C(O1)=O)C(C2(C)C)(C)C)OC)C)=O</chem>
InChI	ATXBJKXCSFZ KBX-FNGWQMIZSA-N
InChIKey	1S/C28H34N2O9/c1-26(2)15-10-7-11-16-20(38-18(11)21(36-6)19(10)39-23(33)17(15)27(26,3)4)22-28(16,5)24(34)29-25(35)30(22)14-8-12(32)13(9-31)37-14/h7,12-17,20,22,31-32H,8-9H2,1-6H3,(H,29,34,35)/t12-,13+,14?,15?,16?,17?,20?,22?,28?/m0/s1