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Typical Product Specifications & Properties

12'-hydroxy-5' α -isobutyl-2'-isopropylergotaman-3',6',18-trione

CAS Number: : 511-09-1

Specifications	Limits
Molecular weight	575.70
EINECS	208-121-2
SMILES	<chem>CC(C)C[C@@H]1N2C(=O)[C@](NC(=O)[C@H]3CN(C)[C@@H]4Cc5c[nH]c6cccc(C4=C3)c56)(O[C@@]2(O)[C@@H]7CCCN7C1=O)C(C)C</chem>
InChI	YDOTUXAWKBPQJW-NSLWYYNWSA-N
InChIKey	1S/C32H41N5O5/c1-17(2)12-25-29(39)36-11-7-10-26(36)32(41)37(25)30(40)31(42-32,18(3)4)34-28(38)20-13-22-21-8-6-9-23-27(21)19(15-33-23)14-24(22)35(5)16-20/h6,8-9,13,15,17-18,20,24-26,33,41H,7,10-12,14,16H2,1-5H3,(H,34,38)/t20-,24-,25+,26+,31-,32+/m1/s1



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