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## Typical Product Specifications & Properties

# (8a)-12'-hydroxy-5'- $\alpha$ -isobutyl-2'-isopropylergotaman-3',6',18-trione

CAS Number: : 511-10-4

| Specifications   | Limits   |
|------------------|--|
| Molecular weight | 575.70   |
| EINECS           | 208-122-8  |
| SMILES           | <chem>CC(C)C[C@@H]1N2C(=O)[C@](NC(=O)[C@@H]3CN(C)[C@@H]4Cc5c[nH]c6ccccc(C4=C3)c56)(O[C@@]2(O)[C@@H]7CCCN7C1=O)C(C)C</chem>   |
| InChI            | YDOTUXAWKBPQJW-JJANYQHSSA-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-/m0/s1 |



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