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Typical Product Specifications & Properties

12'-hydroxy-2',5'- α - diisopropylergotaman-3',6',18- trione phosphate

CAS Number: : 6030-85-9

| Specifications | Limits |
|------------------|--|
| Molecular weight | 641.65 |
| EINECS | 227-906-0 |
| SMILES | <chem>CC(C)[C@H]1C(=O)N2CCC[C@H]2[C@]3(N1C(=O)[C@](O3)(C(C)C)NC(=O)[C@H]4CN([C@@H]5Cc6c[nH]c7c6c(ccc7)C5=C4)C)O.OP(=C(O)O</chem> |
| InChI | YVCZHSXMHRDXIC-CWNVUFIVSA-N |
| InChIKey | 1S/C31H39N5O5.H3O4P/c1-16(2)26-28(38)35-11-7-10-24(35)31(40)36(26)29(39)30(41-31,17(3)4)33-27(37)19-12-21-20-8-6-9-22-25(20)18(14-32-22)13-23(21)34(5)15-19;1-5(2,3)4/h6,8-9,12,14,16-17,19,23-24,26,32,40H,7,10-11,13,15H2,1-5H3,(H,33,37);(H3,1,2,3,4)/t |



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