



www.parchem.com

GET A QUICK QUOTE

Typical Product Specifications & Properties

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

CAS Number: : 2207-69-4

| Specifications | Limits |
|------------------|--|
| Molecular weight | 639.76 |
| EINECS | 218-625-4 |
| SMILES | <chem>C=1[C@H](C[N@@]([C@@H]2Cc3c4c([nH]c3)cccc4C12)C)C(N[C@]1(C(N2[C@@](C(N3CCC[C@@H]3[C@@]2(O1)O)=O)C(C)C)=O)C(C)C)=O.O.C(=O)O</chem> |
| InChI | JSSWJSBxBKEBMS-JDFJKJGNSA-N |
| InChIKey | 1S/C31H39N5O5.CH4O3S/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)19-12-21-20-22-25(20)18(14-32-22)13-23(21)34(5)15-19;1-5(2,3)4/h6,8-9,12,17,19,23-24,26,32,40H,7,10-11,13,15H2,1-5H3,(H,33,37);1H3,(H,2, |



GET A QUICK QUOTE

415 Huguenot Street, New Rochelle, New York 10801