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Typical Product Specifications & Properties

Dihydroergotoxine

CAS Number: : 11032-41-0

| Specifications | Limits |
|------------------|--|
| Molecular weight | 679.78 |
| SMILES | <chem>c1(ccccc1)C[C@@H]1C2[C@]([C@H]3N(CCC3)C1=O)(O[C@@](C2=O)([C@H](C)C)NC(=O)[C@@H]1C[C@H]2[C@H](N(C1)C)Cc1c[nH]c3c1c2ccc3)O.C[C@H]([C@@H]1C2[C@]([C@H]3N(CCC3)C1=O)(O[C@@](C2=O)([C@H](C)C)NC(=O)[C@@H]1C[C@H]2[C@H](N(C1)C)Cc1c[nH]c3c1c2ccc3)O)C.N(C(=O)C1C[</chem> |
| InChI | QHZUABXEBRG BLP-LKWYKXIFSA-N |
| InChIKey | 1S/C36H42N4O5.C33H44N4O5.C32H42N4O5.3CH4O3S/c1-20(2)35(38-33(42)23-16-25-24-11-7-12-27-30(24)22(18-37-27)17-28(25)39(3)19-23)32(41)31-26(15-21-9-5-4-6-10-21)34(43)40-14-8-13-29(40)36(31,44)45-35;1-17(2)12-23-28-29(38)32(18(3)4,42-33(28,41)26-10-7-11-3 |



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