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Typical Product Specifications & Properties

Tertiapin

CAS Number: : 58694-52-3

| Specifications | Limits |
|------------------|--|
| Molecular weight | 2,459.13 |
| SMILES | <chem>N(C([C@@H](NC(=O)[C@@H]1CCCN1C(=O)[C@@H](NC([C@H]([C@H](CC)C)NC([C@H]([C@@H](C)CC)NC(=O)[C@H](CCCNC(N)=N)NC([C@H](CC(N)=O)NC(=O)[C@H](CS)NC(=O)[C@@H](NC(=O)[C@H](CS)NC(=O)[C@H](CC(C)C)NC([C@H](C)N)=O)CC(N)=O)=O)=O)=O)C(CC)CC)Cc1[nH]cnc1)=O)[C@H](C(N[C</chem> |
| InChI | QWKNGDW CZ WKGME-NPHAJLT CSA-N |
| InChIKey | 1S/C106H180N34O23S5/c1-11-56(7)83(137-93(151)68(32-24-39-118-106(115)116)126-97(155)73(45-80(112)141)130-101(159)78(53-167)136-98(156)74(46-81(113)142)131-100(158)77(52-166)135-94(152)70(42-55(5)6)128-87(145)58(9)111)103(161)138-84(57(8)12-2)104(162) |



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