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Typical Product Specifications & Properties

cucurbitacin B

CAS Number: : 6199-67-3

| Specifications | Limits |
|------------------|--|
| Molecular weight | 558.70 |
| SMILES | <chem>CC(=O)OC(C)(C)\C=C\C(=O)[C@](C)(O)[C@H]1[C@H](O)C[C@@]2(C)[C@@H]3CC=C4[C@@H](C[C@H](O)C(=O)C4(C)C)[C@]3(C)C(=O)C[C@]12C</chem> |
| InChI | IXQKXEUSCPEQRD-DKRGWESNSA-N |
| InChIKey | 1S/C32H46O8/c1-17(33)40-27(2,3)13-12-23(36)32(9,39)25-21(35)15-29(6)22-11-10-18-19(14-20(34)26(38)28(18,4)5)31(22,8)24(37)16-30(25,29)7/h10,12-13,19-22,25,34-35,39H,11,14-16H2,1-9H3/b13-12+/t19-,20+,21-,22+,25+,29+,30-,31+,32+/m1/s1 |



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