

1-HYDROXY-14-(2-HYDROXYPROPAN-2-YL)-13-METHYL-4,7,10-TRIOXAPENTACYCLO[6.4.1.1^{9,12}.0^{3,5}.0^{5,13}]]TETRADECANE-6,11-DIONE; [1-HYDROXY-13-METHYL-6-OXO-14-(PROP-1-EN-2-YL)-4,7,10-TRIOXAPENTACYCLO[6.4.1.1^{9,12}.0^{3,5}.0^{5,13}]]TETRADECAN-11-YLIDENE]OXIDANIUM

Catalog Id:

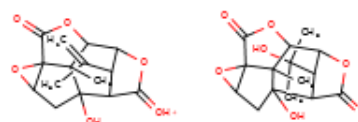
MM124878

IUPAC:

PICROTOXIN

CAS Number:

124-87-8



More Information:

Molecular Weight: 603.596

Formula: C₃₀H₃₅O₁₃

SMILES: CC(=C)C1C2OC(=[OH+])C1C1(O)CC3OC33C(=O)OC2C13C.CC(C)(O)C1C2OC(=O)C1C1(O)CC3OC33C(=O)OC2C13C

Preferred IUPAC Name: 1-HYDROXY-14-(2-HYDROXYPROPAN-2-YL)-13-METHYL-4,7,10-TRIOXAPENTACYCLO[6.4.1.1^{9,12}.0^{3,5}.0^{5,13}]]TETRADECANE-6,11-DIONE; [1-HYDROXY-13-METHYL-6-OXO-14-(PROP-1-EN-2-YL)-4,7,10-TRIOXAPENTACYCLO[6.4.1.1^{9,12}.0^{3,5}.0^{5,13}]]TETRADECAN-11-YLIDENE]OXIDANIUM

InChIKey: InChIKey=VJKUPQSHOVKBCO-UHFFFAOYNA-O