



Formula: C<sub>29</sub>H<sub>46</sub>O<sub>13</sub>

MW: 602.68

CAS: 340169-01-9

MDL: MFCD06668051

TNP: TNP00120

(-)-OUABAIN HYDRATE 98; (-)-OUABAIN HYDRATE 98%



LogP: -0.88

LogS: -2.65

Acceptors: 13

Donors: 10

Rotation Bonds: 1

Chiral Centers: 15

N+O: 13

LIPINSKY: 1

IUPAC: 4-[5-((6S,2R,3R,4R,5R)-3,4,5-trihydroxy-6-methyl(2H-3,4,5,6-tetrahydropyran-2-yloxy))(1S,5S,7S,11S,2R,3R,10R,14R,15R,17R)-3,7,11,17-tetrahydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.0.0.0]heptadec-14-yl]-5-hydrofuran-2-one, hydrate

Smiles:

O1[C@@H](O[C@H]2C[C@H]([C]3([C@@H]4([C@H]([C]5(CC[C@@H]([C]5(C[C@H]4O)C)(C4=CC(=O)OC4))O)(CC[C]3(C2)O)))CO)O)[C@@H]([C@@H]([C@H](O)[C@@H]1C)O)O.O

Specification: (-)-OUABAIN HYDRATE 98 Chemical Properties:

mp 185-192 C(lit.) Safety Information Hazard Codes T Risk Statements 23/25-33 Safety Statements 45 RIDADR UN 1544 6.1/PG 1 (-)-OUABAIN HYDRATE 98 Usage And Synthesis (-)-OUABAIN HYDRATE 98