



Formula: C₂₉H₄₄O₁₂

MW: 584.66

Salt: 8H₂O

CAS: 11018-89-6

MDL NUMBER: MFCD03548271

Smiles:

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O1[C@@H](C)[C@@H]([C@H]([C@H](O)[C@@H]1O[C@H]1C[C@@H](O)[C@@]2(CO)[C@](O)(C1)CC[C@H]1([C]3([C](C[C@H]([C@H]21)O)([C@H](CC3)C1=CC(OC1)=O)C)O))O)O
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Ouabain octahydrate 96%

THERAPEUTIC CATEGORY: Cardiotonic

VET THERAP CATEGORY: Cardiotonic, Diuretic

ACCEPTORS: 12

DONORS: 8

ROTATION BONDS: 1

N+O: 12

Chiral Centers: 15

LogP: -1

LogS: -3.81

LIPINSKI: 1

Synonyms: G-STROPHANTHIN OCTAHYDRATE;G-STROPHANTIN OCTAHYDRATE;STROPHANTHIN G;STROPHANTHIN G, OCTAHYDRATE;OUABAIN 8H2O;OUABAIN 8H2O;OUABAIN HYDRATE;(-)-OUABAIN OCTAHYDRATE

CAS:11018-89-6

MF:C29H60O20

MW:728.77

EINECS:211-139-3

Product Categories: OUABAIN OCTAHYDRATE

Chemical Properties: mp 260 C solubility H2O: 10 mg/mL cold form powder color white T Risk Statements 23/25-33 Safety Statements 45 RIDADR UN 1544 6.1/PG 1 WGK Germany 3 RTECS RN3850000 F 8 HazardClass 6.1(b) PackingGroup III OUABAIN OCTAHYDRATE

Usage And Synthesis:

Chemical Properties: white to off-white crystalline powder OUABAIN OCTAHYDRATE

