

Formula: C19H22O6

MW: 346.38

CAS: 77-06-5

MDL: MFCD01101536

TNP: TNP00129

PRO-GIBB; RELEASE; RYZUPSTRONG; UVEX;

(1alpha,2beta,4aalpha,4bbeta,10beta)-2,4a,7-trihydroxy-1-methyl-8-methylenegibb; (1alpha,2beta,4aalpha,4bbeta,10beta)-2,4a,7-Trihydroxy-1-methyl-8-methylgibb-3-ene-1,10-dic arboxylic acid 1,4a-lactone; (1alpha,2beta,4aalpha,



LogP: -1.28

LogS: -2.66

Acceptors: 6

Donors: 3

Rotation Bonds: 2

Chiral Centers: 8

N+O: 6

LIPINSKY: 4

IUPAC: (1S,3S,4S,7S,14S,2R,10R,11R)-7,14-dihydroxy-1-methyl-6-methylene-15-oxo-16-oxa pentacyclo[9.3.2.1.0.0]heptadec-12-ene-3-carboxylic acid

Smiles:

C(=O)(O)[C@H]1C2C3(C4C51C[C@@](C(C5)=C)(CC4)O)O[C@@](C2(C)C(C=C3)O)=O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(CC4)O(

AGRICULTURE ACTIVITY: Plant growth regulator

SOURCE: Plant hormone; most outstanding of the plantgrowth metabolites of Gibberella fujikuroi.

Specification: FINE Chemical & INTERMEDIATES; Plant Oils, Toxins, Phenolic Acids & Derivatives; Biochemistry; Plant Growth Regulators; Plant Growth Trgulators (Others); Antibiotic Explorer Gibberellic acid Chemical Properties:

mp 227 C alpha 82.5