



Formula: C₄₂H₃₈O₂₀

MW: 862.75

CAS: 128-57-4

MDL: MFCD01109111

TNP: TNP00589



LogP: 3.2

LogS: -4.35

Acceptors: 20

Donors: 12

Rotation Bonds: 11

Chiral Centers: 12

N+O: 20

LIPINSKY: 1

Info: Isolation from Tinnevelly Senna

IUPAC: (9R)-9-[(9S)-5-[(2S,4S,5S,3R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)(2H-3,4,5,6-tetrahydropyran-2-yloxy)]-2-carboxy-4-hydroxy-10-oxo(9-9-hydroanthryl)]-5-[(2S,4S,5S,3R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)(2H-3,4,5,6-tetrahydropyran-2-yloxy)]-4-hydroxy-10-oxo-9-hydroanthracene-2-carboxylic acid

Smiles:

c12C(c3c(O[C@H]4[C@@H]([C@@H](O)[C@@H]([C@H](O4)CO)O)O)cccc3[C@@H]([C@H]3(c4c(c(cc4)C(=O)O)O)C(c4c3cccc4O[C@H]3[C@@H]([C@@H](O)[C@@H]([C@H](O3)CO)

O)O)=O))(c1cc(cc2O)C(=O)O))=O

THERAPEUTIC CATEGORY: Cathartic