



Formula: C22H19O13

MW: 491.39

Salt: Al+++

MDL: MFCD01825026

TNP: TNP00213



LogP: 6.75

LogS: -5.54

Acceptors: 13

Donors: 8

Rotation Bonds: 5

Chiral Centers: 5

N+O: 13

LIPINSKY: 1

IUPAC: 7-[(5S,2R,3R,4R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)(2H-3,4,5,6-tetrahydropyran-2-yl)]-3,5,6,8-tetrahydroxy-1-methyl-9,10-dioxoanthracene-2-carboxylic acid

Smiles:

c1([C@H]2O[C@H](CO)[C@H]([C@@H]([C@H]2O)O)O)c(c2C(c3c(c(C([O-])=O)c(cc3C(c2c(c1O)O)=O)O)C)=O)O