



Formula: C₂₁H₂₈O₁₂

MW: 472.45

CAS: 4773-96-0

MDL: MFCD05618216

TNP: TNP00143



LogP: 1.68

LogS: -3.63

Acceptors: 12

Donors: 12

Rotation Bonds: 8

Chiral Centers: 5

N+O: 12

LIPINSKY: 2

IUPAC: 1,3-dihydroxy-2-[4,5,6-trihydroxy-7-(hydroxymethyl)oxocan-3-yl]xanthen-9-one, hydrate, hydrate, hydrate

Smiles: c12c(c3ccccc3oc2cc(O)c(c1O)C1C(C(C(O)C(COC1)CO)O)O)=O.O.O.O.O