



Formula: C₁₂H₂₂O₁₁

MW: 342.3

MDL: MFCD01873927

TNP: TNP00417



LogP: 1.47

LogS: -3.68

Acceptors: 11

Donors: 8

Rotation Bonds: 3

Chiral Centers: 10

N+O: 11

LIPINSKY: 2

Info: D(+)-Cellobiose 98%, Preparation from cotton. Does not occur free in nature

IUPAC: (3S,4S,6S,5R)-5-[(4S,5S,2R,3R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)(2H-3,4,5,6-tetrahydropyran-2-yl)oxy]-6-(hydroxymethyl)-2H-3,4,5,6-tetrahydropyran-2,3,4-triol

Smiles:

C([C@@H]1[C@@H](O)[C@@H]([C@H]([C@H](O1)O)[C@@H]1[C@H]([C@H](O)C(O[C@H]1CO)O)O)O)O