



Formula: C<sub>13</sub>H<sub>18</sub>O<sub>7</sub>

MW: 286.28

CAS: 138-52-3

MDL: MFCD00078363

TNP: TNP00398

SALICYLALDEHYDE-B-D-GLUCOSIDE; SALICYLALCOHOL BETA-D-GLUCOSIDE; SALICYL ALCOHOL GLUCOSIDE; SALICOSIDE; SALICIN; SALIGENIN-B-D-GLUCOSIDE; SALIGENIN-B-D-GLYCOPYRANOSIDE; WHITE WILLOW



LogP: 2.87

LogS: -3.96

Acceptors: 7

Donors: 5

Rotation Bonds: 4

Chiral Centers: 5

N+O: 7

LIPINSKY: 4

Info: D(-)-Salicin 99+%

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

Smiles: O1[C@@H](Oc2ccccc2CO)[C@H](O)[C@@H](O)[C@@H]([C@H]1CO)O

Specification: Sugars, Carbohydrates & Glucosides; Biochemistry; Glucose; Glycosides;  
Sugars; Natural Plant Extract; Herbs & Natural Remedies  
2-(Hydroxymethyl)phenyl-beta-D-glucopyranoside Chemical Properties:

mp 196-202 C alpha -61.5