



Formula: C₁₂H₂₂O₁₁

MW: 342.3

CAS: 554-91-6

MDL: MFCD02667799

TNP: TNP00402

6-O-BETA-D-GLUCOPYRANOSYL-D-GLUCOPYRANOSE; B-GENTIOBIOSE;
BETA-GENTIOBIOSE; BETA-D-GENTIOBIOSE; GENTIOBIOSE; GENTIOBIOSE, B-(RG)



LogP: -8.56

LogS: -3.89

Acceptors: 11

Donors: 8

Rotation Bonds: 2

Chiral Centers: 10

N+O: 11

LIPINSKY: 2

Info: Gentiobiose 97%

IUPAC: (4S,5S,2R,3R,6R)-6-[[[(4S,5S,2R,3R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)(2H-3,4,5,6-tetrahydropyran-2-yloxy)]methyl]-2H-3,4,5,6-tetrahydropyran-2,3,4,5-tetr aol

Smiles:

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

@H]1O)O)O)O)O)O

Specification: 6-O-BETA-D-GLUCOPYRANOSYL-D-GLUCOPYRANOSE Chemical Properties:

Safety 24/25 6-O-BETA-D-GLUCOPYRANOSYL-D-GLUCOPYRANOSE Usage And Synthesis 6-O-BETA-D-GLUCOPYRANOSYL-D-GLUCOPYRANOSE

Merck 13 Reference: Monograph Number: 0004407

Title: Gentiobiose

CAS Registry Number: 554-91-6

CAS Name: 6-O-b-D-Glucopyranosyl-D-glucose

Additional Names: 6-(b-D-glucosido)-D-glucose; amygdalose

Molecular Formula: C₁₂H₂₂O₁₁

Molecular Weight: 342.30.

Percent Composition: C 42.11%, H 6.48%, O 51.41%

Literature References: From gentianose by partial hydrolysis with 0.2% H₂SO₄ or with invertin. From D-glucose by enzymatic synthesis with emulsin: Helferich, Lette, Org. Synth. 22, 53 (1942). Prepn and structure: Haworth, Wylam, J. Chem. Soc. 123, 3120 (1923); Hudson, J. Am. Chem. Soc. 51, 1708 (1930). Structure: Hassid, Ballou in W. Pigman, The Carbohydrates (Academic Press, New York, 1957) p 492. Synthesis: Helferich, Klein, Ann. 450, 219 (1926); Reynolds, Evans, J. Am. Chem. Soc. 60, 2559 (1938). Hydrolysis with almond emulsin gives 2 mols D-glucose.

Derivative Type: a-Form

Properties: Lentil-shaped crystals with 2CH₃OH from methanol. Bitter taste. Very hygroscopic. mp 86. Shows mutarotation. [α]_D²² +16 (3 min)