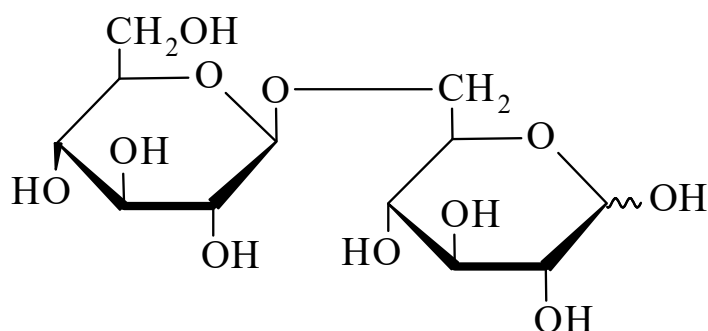




>>Entry Name: 6-*O*-β-D-Glucopyranosyl-D-glucose, 9Cl

ENTRY UNDER REVIEW

Synonym(s): Gentiobiose, 8Cl. Amygdalose



CAS Registry Number: 554-91-6

Molecular Formula: C₁₂H₂₂O₁₁

Molecular Weight: 342.299

Accurate Mass: 342.116215

Percentage Composition: C 42.11%; H 6.48%; O 51.42%

Biological Source: Formed by the hydrol. of Gentiatibetine [GQD53-A](#), Crocetin [JQK77-A](#) and 2-Hydroxy-2-phenylacetonitrile [JDX91-A](#). Occurs free in roots of *Gentiana* spp. and a few other plants, prod. by *Acetobacter* spp.

Fluka: 48790

Sigma: G3000

>>Derivative: Phenylsazone

Molecular Formula: C₂₄H₃₂N₄O₉

Molecular Weight: 520.538

Percentage Composition: C 55.38%; H 6.20%; N 10.76%; O 27.66%

Melting Point: Mp 184-186° (162-167° dec.)

Optical Rotation: $[\alpha]_D^{20} -14.8$ (Py)

>>Derivative: 1-*O*-(3,4-Dihydroxycinnamoyl)

Synonym(s): 1-*O*-Caffeoylgentiobiose

Molecular Formula: C₂₁H₂₈O₁₄

Molecular Weight: 504.444

Accurate Mass: 504.14791

Percentage Composition: C 50.00%; H 5.59%; O 44.40%

Biological Source: Isol. from flowers of *Petunia hybrida*

Other Data: Anomeric config. not detd.

>>Variant: α-Pyranose-form

CAS Registry Number: 5995-99-3

Molecular Formula: C₁₂H₂₂O₁₁

Molecular Weight: 342.299

Accurate Mass: 342.116215

Percentage Composition: C 42.11%; H 6.48%; O 51.42%

Melting Point: Mp 189-195° (anhyd.)

Optical Rotation: $[\alpha]_D +31 \rightarrow +9.6$ (H₂O)

>>Derivative: Octa-Ac

Synonym(s): Octa-*O*-acetyl-α-gentiobiose

Molecular Formula: C₂₈H₃₈O₁₉

Molecular Weight: 678.597

Accurate Mass: 678.200735

Percentage Composition: C 49.56%; H 5.64%; O 44.80%

Melting Point: Mp 188-189°

Optical Rotation: $[\alpha]_D^{20} +52.3$ (CHCl₃)