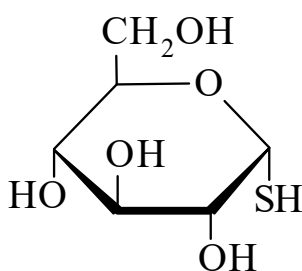




>>Entry Name: 1-Thiogluucose, 9Cl, 8Cl

Synonym(s): Glucothiose



α-Pyranose-form

Molecular Formula: C₆H₁₂O₅S

Molecular Weight: 196.224

Accurate Mass: 196.040545

Percentage Composition: C 36.73%; H 6.16%; O 40.77%; S 16.34%

Biological Source: Occurs widely in plants in a variety of complex glycosides from which it can usually be obt. by alkaline hydrol.

>>Variant: D-form

CAS Registry Number: 7211-44-1

Molecular Formula: C₆H₁₂O₅S

Molecular Weight: 196.224

Accurate Mass: 196.040545

Percentage Composition: C 36.73%; H 6.16%; O 40.77%; S 16.34%

Physical Description: Amorph. solid + 1H₂O. Forms crystalline salts

>>Derivative: Na salt

CAS Registry Number: 10593-29-0

Physical Description: Cryst. +2H₂O

Melting Point: Mp 173 dec.°

Optical Rotation: [α]_D +18 (H₂O) (+14.1)

Sigma: T6375

>>Variant: α -D-Pyranose-form

Molecular Formula: C₆H₁₂O₅S

Molecular Weight: 196.224

Accurate Mass: 196.040545

Percentage Composition: C 36.73%; H 6.16%; O 40.77%; S 16.34%

>>Derivative: O,O,O,O,S-Penta-Ac

Synonym(s): 1,2,3,4,6-Pentaacetyl-1-thio- α -D-glucopyranose. 2,3,4,6-Tetra-O-acetyl-1-S-acetyl-1-thio- α -D-glucopyranose

Molecular Formula: C₁₆H₂₂O₁₀S

Molecular Weight: 406.41

Accurate Mass: 406.09337

Percentage Composition: C 47.29%; H 5.46%; O 39.37%; S 7.89%

Physical Description: Cryst. (Et₂O/pentane or EtOH)

Melting Point: Mp 123-125°

Optical Rotation: [α]_D +143.5 (c, 1.95 in CHCl₃)

>>Derivative: Me glycoside

Synonym(s): Methyl 1-thio- α -D-glucopyranoside

Molecular Formula: C₇H₁₄O₅S

Molecular Weight: 210.251

Accurate Mass: 210.056195

Percentage Composition: C 39.99%; H 6.71%; O 38.05%; S 15.25%

Physical Description: Needles (EtOAc)

Melting Point: Mp 137°

Optical Rotation: [α]_D³⁰ +124.5 (H₂O)