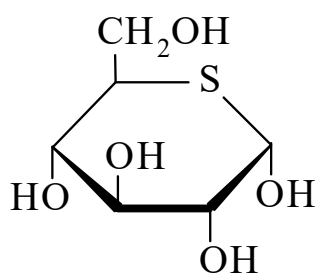




>>Entry Name: 5-Thioglucose, 9Cl, 8Cl



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%

>>Variant: D-Pyranose-form

CAS Registry Number: 16505-91-2

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%

Use/Importance: Interferes with spermatogenesis; exhibits diabetogenic activity in rats; effective against malignant cultured cells

Physical Description: Needles (CHCl₃/MeOH)

Melting Point: Mp 135-136°

Optical Rotation: [α]_D²⁰+188 (c, 1.56 in H₂O)

>>Variant: α-D-Pyranose-form

CAS Registry Number: 20408-97-3

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%

Aldrich: 85986-9

Fluka: 88635

Sigma: T2635

>>Derivative: Penta-Ac

Synonym(s): 1,2,3,4,6-Penta-*O*-acetyl-5-thio-α-D-glucopyranose

CAS Registry Number: 10227-18-6

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%

Melting Point: Mp 103°

Optical Rotation: [α]_D²³+213 (c, 1.56 in CHCl₃)

>>Derivative: Me glycoside

Synonym(s): Methyl 5-thio-α-D-glucopyranoside

CAS Registry Number: 28585-88-8

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: Cryst. (MeOH)

Melting Point: Mp 126°

Optical Rotation: [α]_D²⁵+326.3 (c, 1.61 in MeOH)