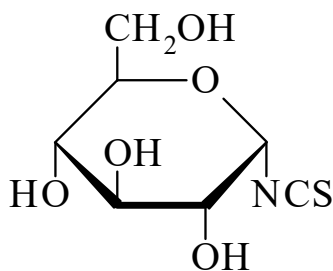




>>Entry Name: Glucopyranosyl isothiocyanate



α -D-form

Related CAS Registry Numbers(s): 18866-59-6

Molecular Formula: C₇H₁₁NO₅S

Molecular Weight: 221.234

Accurate Mass: 221.035794

Percentage Composition: C 38.00%; H 5.01%; N 6.33%; O 36.16%; S 14.49%

>>Variant: α -D-form

Molecular Formula: C₇H₁₁NO₅S

Molecular Weight: 221.234

Accurate Mass: 221.035794

Percentage Composition: C 38.00%; H 5.01%; N 6.33%; O 36.16%; S 14.49%

>>Derivative: Tetra-Ac

Synonym(s): 2,3,4,6-Tetra-*O*-acetyl- α -D-glucopyranosyl isothiocyanate

Molecular Formula: C₁₅H₁₉NO₉S

Molecular Weight: 389.382

Accurate Mass: 389.078054

Percentage Composition: C 46.27%; H 4.92%; N 3.60%; O 36.98%; S 8.24%

Melting Point: Mp 92-94°

Optical Rotation: [α]_D +114.5 (CHCl₃)

>>Variant: β -D-form

Molecular Formula: C₇H₁₁NO₅S

Molecular Weight: 221.234

Accurate Mass: 221.035794

Percentage Composition: C 38.00%; H 5.01%; N 6.33%; O 36.16%; S 14.49%

>>Derivative: Tetra-Ac

Synonym(s): 2,3,4,6-Tetra-*O*-acetyl- β -D-glucopyranosyl isothiocyanate. TAGIT

CAS Registry Number: 14152-97-7

Molecular Formula: C₁₅H₁₉NO₉S

Molecular Weight: 389.382

Accurate Mass: 389.078054

Percentage Composition: C 46.27%; H 4.92%; N 3.60%; O 36.98%; S 8.24%

Use/Importance: Derivatisation reagent for the resolu. of amino acids by hplc

Melting Point: Mp 112-113°

Optical Rotation: [α]_D +5 (c, 1 in CHCl₃)

Aldrich: 33858-3

Fluka: 86550

Sigma: T5783

References:

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Muller, A. *et al.*, *Ber.*, 1941, **74**, 698, (*synth*)

Nimura, N. *et al.*, *J. Chromatogr.*, 1980, **202**, 375; 1981, **210**, 77; 1984, **316**, 547, (*use*)

Gal, J. *et al.*, *J. Liq. Chromatogr.*, 1984, **7**, 2307; 1986, **9**, 673, (*use*)

Camarasa, M.J., *Synthesis*, 1984, 509, (*synth*)

Lindhorst, T.K. *et al.*, *Synthesis*, 1995, 1228, (α -Tetra Ac *pmr*, *cmr*)