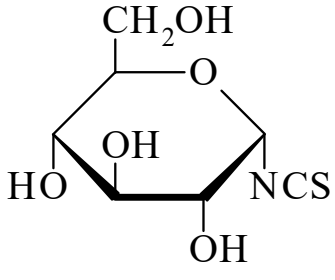
>>**Entry Name: Glucopyranosyl isothiocyanate**



a-D-*form*

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

Molecular Formula: $C_7H_{11}NO_5S$
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: $C_7H_{11}NO_5S$
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: $C_{15}H_{19}NO_9S$
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: $[\alpha]_D$ +114.5 ($CHCl_3$)

>>**Variant:** β-D-form

Molecular Formula: $C_7H_{11}NO_5S$
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: $C_{15}H_{19}NO_9S$
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 resoln. of amino acids by hplc
Melting Point: Mp 112-113°
Optical Rotation: $[\alpha]_D$ +5 (c, 1 in $CHCl_3$)
Aldrich: 33858-3
Fluka: 86550
Sigma: T5783

References:

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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)*