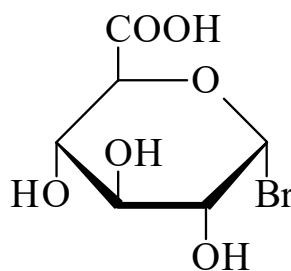




>>Entry Name: Glucopyranosyluronic acid bromide



Molecular Formula: C₆H₉BrO₆

Molecular Weight: 257.037

Accurate Mass: 255.978251

Percentage Composition: C 28.04%; H 3.53%; Br 31.09%; O 37.35%

>>Variant: α-D-Pyranose-form

Molecular Formula: C₆H₉BrO₆

Molecular Weight: 257.037

Accurate Mass: 255.978251

Percentage Composition: C 28.04%; H 3.53%; Br 31.09%; O 37.35%

>>Derivative: Tri-Ac, Me ester

Synonym(s): Methyl 2,3,4-tri-*O*-acetyl-1-bromo-1-deoxy-α-D-glucopyranuronate, 8Cl. Methyl (2,3,4-tri-*O*-acetyl-α-D-glucopyranosyl)uronate bromide

CAS Registry Number: 21085-72-3

Molecular Formula: C₁₃H₁₇BrO₉

Molecular Weight: 397.176

Accurate Mass: 396.025596

Percentage Composition: C 39.31%; H 4.31%; Br 20.12%; O 36.25%

Use/Importance: Glycosidation reagent in synth. of glucuronides

Physical Description: Cryst. (EtOH)

Melting Point: Mp 106-107°

Optical Rotation: [α]_D²⁵+197 (c, 1 in CHCl₃)

Fluka: 533

Sigma: A8292

>>Variant: β-D-Pyranose-form

Molecular Formula: C₆H₉BrO₆

Molecular Weight: 257.037

Accurate Mass: 255.978251

Percentage Composition: C 28.04%; H 3.53%; Br 31.09%; O 37.35%

>>Derivative: Tri-Ac, Me ester

Synonym(s): Methyl 2,3,4-tri-*O*-acetyl-1-bromo-1-deoxy-β-D-glucopyranuronate. Methyl (2,3,4-tri-*O*-acetyl-β-D-glucopyranosyl)uronate bromide

Molecular Formula: C₁₃H₁₇BrO₉

Molecular Weight: 397.176

Accurate Mass: 396.025596

Percentage Composition: C 39.31%; H 4.31%; Br 20.12%; O 36.25%

Physical Description: Cryst.

Melting Point: Mp 138-140°

Optical Rotation: [α]_D²⁰-22 (c, 5.1 in C₆H₆)

References:

Bollenback, G.N. *et al.*, *J.A.C.S.*, 1955, **77**, 3310, (*synth*)

Heyns, K. *et al.*, *Chem. Ber.*, 1966, **99**, 1183, (*synth*)

Emiliozzi, R., *Bull. Soc. Chim. Fr.*, 1968, 738, (*synth*)

Doherty, R.M. *et al.*, *Carbohydr. Res.*, 1983, **116**, 150, (*cryst struct*)