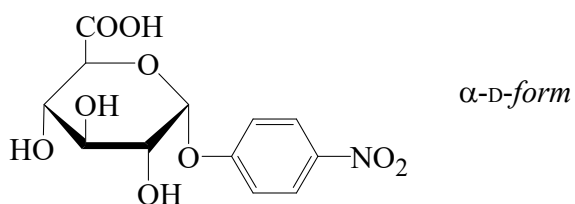




>>Entry Name: 4-Nitrophenyl glucopyranosiduronic acid



Molecular Formula: C₁₂H₁₃NO₉

Molecular Weight: 315.236

Accurate Mass: 315.059034

Percentage Composition: C 45.72%; H 4.16%; N 4.44%; O 45.68%

Sigma: N7896

>>Variant: α -D-form

CAS Registry Number: 71484-85-0

Molecular Formula: C₁₂H₁₃NO₉

Molecular Weight: 315.236

Accurate Mass: 315.059034

Percentage Composition: C 45.72%; H 4.16%; N 4.44%; O 45.68%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 211-212° (dec.)

Optical Rotation: [α]_D +161 (c, 1.0 in EtOH)

>>Variant: β -D-form

CAS Registry Number: 10344-94-2

Molecular Formula: C₁₂H₁₃NO₉

Molecular Weight: 315.236

Accurate Mass: 315.059034

Percentage Composition: C 45.72%; H 4.16%; N 4.44%; O 45.68%

Use/Importance: Substrate for assay of β -glucuronidase activity

Physical Description: Cryst. (EtOAc/Et₂O aq.)

Melting Point: Mp 139°

Optical Rotation: [α]_D²⁴ -108 (c, 1 in EtOH)

Other Data: Hygroscopic; forms a monohydrate (Mp 95°) in air

Sigma: N1627

>>Derivative: Tri-Ac, Me ester

CAS Registry Number: 18472-49-6

Molecular Formula: C₁₉H₂₁NO₁₂

Molecular Weight: 455.374

Accurate Mass: 455.106379

Percentage Composition: C 50.11%; H 4.65%; N 3.08%; O 42.16%

Physical Description: Cryst. (EtOH) or needles (MeOH)

Melting Point: Mp 153-154°

Optical Rotation: [α]_D²⁵ -52.1 (c, 1 in CHCl₃)

Sigma: M5002

References:

Marsh, C.A. *et al.*, *Biochem. J.*, 1958, **68**, 617-621, (*synth*)

Kato, K. *et al.*, *Chem. Pharm. Bull.*, 1960, **8**, 239-242, (β -D-*form*)

Weintraub, L. *et al.*, *J.C.S.(C)*, 1969, 1562-1564, (β -D-*tri-Ac Me ester*)

Asen, S. *et al.*, *Phytochemistry*, 1974, **13**, 1219-1223, (*derivs, pmr, ir*)

Kiss, J. *et al.*, *Helv. Chim. Acta*, 1975, **58**, 301-310, (*derivs, synth, pmr*)

Honma, K. *et al.*, *Chem. Pharm. Bull.*, 1976, **24**, 394-399, (β -D-*form, synth, ir, pmr, ord*)

Johnson, L.P. *et al.*, *Carbohydr. Res.*, 1979, **73**, 255-259, (β -D-*form, synth, pmr, cmr*)