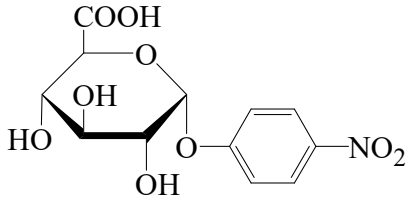
>>**Entry Name: 4-Nitrophenyl glucopyranosiduronic acid**



α-D-*form*

Molecular Formula: $C_{12}H_{13}NO_9$
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: $C_{12}H_{13}NO_9$
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: $[\alpha]_D$ +161 (c, 1.0 in EtOH)

>>**Variant:** β-D-form

CAS Registry Number: 10344-94-2

Molecular Formula: $C_{12}H_{13}NO_9$
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/Et_2O aq.)
Melting Point: Mp 139°
Optical Rotation: $[\alpha]_D^{24}$ –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: $C_{19}H_{21}NO_{12}$
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: $[\alpha]_D^{25}$ –52.1 (c, 1 in $CHCl_3$)
Sigma: M5002

References:

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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)*

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