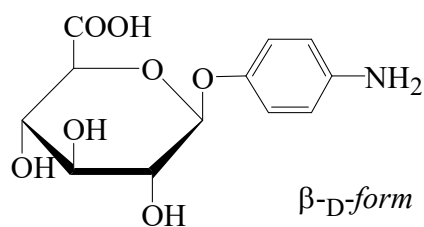




>>Entry Name: 4-Aminophenyl glucopyranosiduronic acid



Molecular Formula: C₁₂H₁₅NO₇

Molecular Weight: 285.253

Accurate Mass: 285.084854

Percentage Composition: C 50.53%; H 5.30%; N 4.91%; O 39.26%

>>Variant: β -D-form

CAS Registry Number: 21080-66-0

Molecular Formula: C₁₂H₁₅NO₇

Molecular Weight: 285.253

Accurate Mass: 285.084854

Percentage Composition: C 50.53%; H 5.30%; N 4.91%; O 39.26%

Physical Description: Cryst. + 1H₂O (H₂O)

Melting Point: Mp 213° (monohydrate)

Optical Rotation: $[\alpha]_D^{25}$ -83 (c, 1 in 0.1N HCl)

>>Derivative: N-Ac

Synonym(s): Paracetamol glucuronide

CAS Registry Number: 16110-10-4

Molecular Formula: C₁₄H₁₇NO₈

Molecular Weight: 327.29

Accurate Mass: 327.095419

Percentage Composition: C 51.38%; H 5.24%; N 4.28%; O 39.11%

Metabolism: Urinary metabolite of [FFL96-T](#)

Physical Description: Cryst. + 1H₂O (MeOH)

Melting Point: Mp 134-136° (monohydrate)

Optical Rotation: $[\alpha]_D^{23}$ -90 (c, 0.16 in H₂O)

References:

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Weintraub, L. *et al.*, *J.C.S.(C)*, 1969, 1562-1564, (*synth*, N-Ac)

Shibasaki, J. *et al.*, *Chem. Pharm. Bull.*, 1970, **18**, 2340-2343, (N-Ac)

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