



Molecular Weight: 213.235
Accurate Mass: 213.078979
Percentage Composition: C 73.23%; H 5.20%; N 6.57%; O 15.01%

Aldrich: 37772-4
Fluka: 72351
Rare Chemicals Library: S57945-9

>>Derivative: Ph ester

CAS Registry Number: 3468-53-9
Molecular Formula: C₁₂H₉NO₂
Molecular Weight: 199.209
Accurate Mass: 199.063329
Percentage Composition: C 72.35%; H 4.55%; N 7.03%; O 16.06%
Physical Description: Cryst. (EtOH)
Melting Point: Mp 71°
Rare Chemicals Library: S37035-5

>>Derivative: 2-Butoxyethyl ester

>>Derivative: β-D-Glucopyranosyl ester
Synonym(s): 1-*O*-Nicotinoyl-β-D-glucopyranose

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%
Biological Source: Present in tobacco (*Nicotiana tabacum*) cells grown in a high conc. of niacin
UV: [neutral] λ_{max} 263 (log ε 3.22) (H₂O)
Other Data: Prob. a detoxification form of niacin in the plant

>>Derivative: Chloride

CAS Registry Number: 10400-19-8
Molecular Formula: C₆H₄ClNO
Molecular Weight: 141.556
Accurate Mass: 140.998141
Percentage Composition: C 50.91%; H 2.85%; Cl 25.04%; N 9.89%; O 11.30%
Physical Description: Cryst.
Melting Point: Mp 15-16°
Boiling Point: Bp₁₂ 85°

>>Derivative: Chloride; hydrochloride

CAS Registry Number: 20260-53-1
Melting Point: Mp 155.5-156.5°
Other Data: Sublimes
Aldrich: 21338-1

>>Derivative: Amide

>>Derivative: Anilide

CAS Registry Number: 1752-96-1
Molecular Formula: C₁₂H₁₀N₂O
Molecular Weight: 198.224
Accurate Mass: 198.079313
Percentage Composition: C 72.71%; H 5.08%; N 14.13%; O 8.07%
Physical Description: Cryst. + 2H₂O (H₂O)
Melting Point: Mp 85°
Aldrich: 45482-6
Rare Chemicals Library: S37724-4