



Molecular Weight: 179.175
Accurate Mass: 179.058244
Percentage Composition: C 60.33%; H 5.06%; N 7.82%; O 26.79%
Use/Importance: Tuberculostatic agent
Physical Description: Needles
Melting Point: Mp 256.5°
Calculated Log P Data: Log P 1.2 (calc)
Aldrich: 13333-7
Fluka: 230
Sigma: A3274

>>Derivative: *N*-Benzoyl

CAS Registry Number: 582-80-9
Molecular Formula: C₁₄H₁₁NO₃
Molecular Weight: 241.246
Accurate Mass: 241.073894
Percentage Composition: C 69.70%; H 4.60%; N 5.81%; O 19.90%
Physical Description: Needles (EtOH)
Melting Point: Mp 278°

>>Derivative: *N*-*tert*-Butyloxycarbonyl

CAS Registry Number: 66493-39-8
Molecular Formula: C₁₂H₁₅NO₄
Molecular Weight: 237.255
Accurate Mass: 237.100109
Percentage Composition: C 60.75%; H 6.37%; N 5.90%; O 26.97%
Physical Description: Solid

>>Derivative: *N*-Me

Synonym(s): 4-(Methylamino)benzoic acid

CAS Registry Number: 10541-83-0
Molecular Formula: C₈H₉NO₂
Molecular Weight: 151.165
Accurate Mass: 151.063329
Percentage Composition: C 63.57%; H 6.00%; N 9.27%; O 21.17%
Physical Description: Cryst. (EtOH aq. or C₆H₆)
Melting Point: Mp 168° (155-157°)
Aldrich: 11969-5
Fluka: 65646