



Rare Chemicals Library: S55987-3

>>Derivative: *N*-Ac

Synonym(s): Acedoben, INN

CAS Registry Number: 556-08-1

Molecular Formula: C₉H₉NO₃

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

>>Derivative: *N*-Me, Me ester

CAS Registry Number: 18358-63-9

Molecular Formula: C₉H₁₁NO₂

Molecular Weight: 165.191

Accurate Mass: 165.078979

Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%

Physical Description: Plates (EtOH aq.)

Melting Point: Mp 95.5°

pKa Value: pK_a 11.68 (25°)

Rare Chemicals Library: S94326-6