



Molecular Weight: 165.194
Accurate Mass: 165.090212
Percentage Composition: C 58.17%; H 6.71%; N 25.44%; O 9.69%
Physical Description: Leaflets (EtOH)
Melting Point: Mp 126.5°

>>Derivative: Nitrile

Synonym(s): Anilinoacetonitrile. *N*-(Cyanomethyl)aniline

CAS Registry Number: 3009-97-0
Molecular Formula: C₈H₈N₂
Molecular Weight: 132.165
Accurate Mass: 132.068748
Percentage Composition: C 72.70%; H 6.10%; N 21.20%
Physical Description: Plates (petrol/Et₂O)
Melting Point: Mp 48°

>>Derivative: *N*-Ac

Synonym(s): *N*-Phenylaceturic acid

CAS Registry Number: 579-98-6
Molecular Formula: C₁₀H₁₁NO₃
Molecular Weight: 193.202
Accurate Mass: 193.073894
Percentage Composition: C 62.17%; H 5.74%; N 7.25%; O 24.84%
Physical Description: Leaflets (H₂O)
Melting Point: Mp 194°

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

Molecular Formula: C₁₁H₁₃NO₃
Molecular Weight: 207.229
Accurate Mass: 207.089544
Percentage Composition: C 63.76%; H 6.32%; N 6.76%; O 23.16%
Physical Description: Prisms (petrol)
Melting Point: Mp 59-60°

>>Derivative: *N*-Ac, Et ester

Molecular Formula: C₁₂H₁₅NO₃
Molecular Weight: 221.255
Accurate Mass: 221.105194
Percentage Composition: C 65.14%; H 6.83%; N 6.33%; O 21.69%
Physical Description: Leaflets (EtOH)
Melting Point: Mp 194-195°

>>Derivative: *N*-Benzoyl

Synonym(s): *N*-Phenylhippuric acid

CAS Registry Number: 119656-49-4
Molecular Formula: C₁₅H₁₃NO₃
Molecular Weight: 255.273
Accurate Mass: 255.089544
Percentage Composition: C 70.58%; H 5.13%; N 5.49%; O 18.80%
Physical Description: Amorph.
Melting Point: Mp 63°

>>Derivative: *N*-Me

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1180A, (*nmr*)
Passeron, S. *et al.*, *Bull. Soc. Chim. Fr.*, 1963, 35, (*synth*)