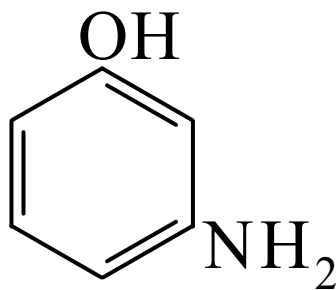




>>Entry Name: **3-Aminophenol**, 9CI

Synonym(s): 1-Amino-3-hydroxybenzene. *m*-Hydroxyaniline



CAS Registry Number: 591-27-5

Related CAS Registry Numbers(s): 101012-81-1

Extra CAS Registry Numbers(s): 27598-85-2

Molecular Formula: C₆H₇NO

Molecular Weight: 109.127

Accurate Mass: 109.052764

Percentage Composition: C 66.04%; H 6.47%; N 12.84%; O 14.66%

Source/Synthesis: Produced by caustic fusion of 3-Aminobenzenesulfonic acid [FFQ92-O](#) or by reduction of 3-Nitrophenol [DTX70-N](#)

Use/Importance: Reagent for hplc anal. of 2-Acetoxybenzoic acid [BLS47-M](#). Used in hair dyes. Monomer for polyester-amides, phenolic resins, and other polymers

Physical Description: Prisms (toluene)

Melting Point: Mp 124-126°

Boiling Point: Bp₁₁ 164°

pKa Value: pK_{a1} 4.37; pK_{a2} 9.82 (20°, 0.1M KCl)

Hazard & Toxicity: Skin and eye irritant. LD₅₀ (rat, orl) 924 mg/kg

Aldrich: 10024-2

Fluka: 9130

>>Derivative: Hydrochloride

CAS Registry Number: 51-81-0

Physical Description: Prisms (H₂O)

Melting Point: Mp 229°

>>Derivative: *N*-Formyl

Synonym(s): 3-Formamidophenol. 3-Hydroxyformanilide. *N*-(3-Hydroxyphenyl)formamide

CAS Registry Number: 24891-35-8

Molecular Formula: C₇H₇NO₂

Molecular Weight: 137.138

Accurate Mass: 137.047679

Percentage Composition: C 61.31%; H 5.14%; N 10.21%; O 23.33%

Melting Point: Mp 116° (110°)

>>Derivative: *N*-Ac

Synonym(s): 3-Acetamidophenol. 3-Hydroxyacetanilide. **Metacetamol**, BAN, INN. BS 749

CAS Registry Number: 621-42-1

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%

Biological Use/Importance: Analgesic

Physical Description: Needles (H₂O)

Development Status: Never marketed

Melting Point: Mp 148-149°

pKa Value: pK_a 9.59 (25°)

Calculated Log P Data: Log P 0.49 (calc)

Hazard & Toxicity: LD₅₀ (mus, ipr) 1025 mg/kg

Aldrich: A720-5

Fluka: 350

Sigma: A4911