



Molecular Formula: C₇H₆ClNO
Molecular Weight: 155.583
Accurate Mass: 155.013791
Percentage Composition: C 54.04%; H 3.89%; Cl 22.79%; N 9.00%; O 10.28%
Physical Description: Yellow cryst.
Melting Point: Mp 31°
Boiling Point: Bp₁₂ 120°

>>Derivative: Amide

CAS Registry Number: 2835-68-9
Molecular Formula: C₇H₈N₂O
Molecular Weight: 136.153
Accurate Mass: 136.063663
Percentage Composition: C 61.75%; H 5.92%; N 20.57%; O 11.75%
Physical Description: Light yellow cryst. + ½H₂O
Melting Point: Mp 183°
Aldrich: 28457-2
Sigma: A1658

>>Derivative: Anilide

Synonym(s): 4-Amino-*N*-phenylbenzamide

CAS Registry Number: 782-45-6
Molecular Formula: C₁₃H₁₂N₂O
Molecular Weight: 212.251
Accurate Mass: 212.094963
Percentage Composition: C 73.57%; H 5.70%; N 13.20%; O 7.54%
Physical Description: Cryst. (C₆H₆/petrol)
Melting Point: Mp 138-140°
pKa Value: pK_a 2.94 (23°, 1.6% MeCN aq.)

>>Derivative: Hydrazide

CAS Registry Number: 5351-17-7
Molecular Formula: C₇H₉N₃O
Molecular Weight: 151.168
Accurate Mass: 151.074562
Percentage Composition: C 55.62%; H 6.00%; N 27.80%; O 10.58%
Use/Importance: Monomer for polyhydrazides
Melting Point: Mp 225-227°

Aldrich: A4190-9

Sigma: A0890

>>Derivative: Nitrile

Synonym(s): 4-Aminobenzonitrile, 9Cl. *p*-Cyanoaniline

CAS Registry Number: 873-74-5
Molecular Formula: C₇H₆N₂
Molecular Weight: 118.138
Accurate Mass: 118.053098
Percentage Composition: C 71.17%; H 5.12%; N 23.71%
Physical Description: Prisms
Melting Point: Mp 86°
pKa Value: pK_a 1.71 (25°, H₂O)
Hazard & Toxicity: LD₅₀ (mus, orl) 650 mg/kg

Aldrich: 14775-3

Fluka: 7010