



Physical Description: Pungent oil

Boiling Point: Bp_{0.5} 110-113°

Hazard & Toxicity: Irritant

>>Derivative: Amide

CAS Registry Number: 618-49-5

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%

Physical Description: Plates (H₂O)

Melting Point: Mp 170.5°

pKa Value: pK_{a1} 9.3 (25°)

>>Derivative: Anilide

CAS Registry Number: 27559-45-1

Molecular Formula: C₁₃H₁₁NO₂

Molecular Weight: 213.235

Accurate Mass: 213.078979

Percentage Composition: C 73.23%; H 5.20%; N 6.57%; O 15.01%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 154-155°

>>Derivative: Hydrazide

CAS Registry Number: 5818-06-4

Molecular Formula: C₇H₈N₂O₂

Molecular Weight: 152.152

Accurate Mass: 152.058578

Percentage Composition: C 55.26%; H 5.30%; N 18.41%; O 21.03%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 157-159°

Aldrich: 46801-0

Other: PB H09761

>>Derivative: Nitrile

Synonym(s): 3-Hydroxybenzonitrile. 3-Cyanophenol

CAS Registry Number: 873-62-1

Molecular Formula: C₇H₅NO

Molecular Weight: 119.123

Accurate Mass: 119.037114

Percentage Composition: C 70.58%; H 4.23%; N 11.76%; O 13.43%

Physical Description: Plates (H₂O)

Melting Point: Mp 82°

pKa Value: pK_a 8.61 (25°)

Aldrich: C9380-0

Fluka: 54796

>>Derivative: Ac

Synonym(s): 3-Acetoxybenzoic acid

CAS Registry Number: 6304-89-8

Molecular Formula: C₉H₈O₄

Molecular Weight: 180.16

Accurate Mass: 180.04226

Percentage Composition: C 60.00%; H 4.48%; O 35.52%

Physical Description: Cryst. (xylene)

Melting Point: Mp 131.5°

Rare Chemicals Library: S91432-0