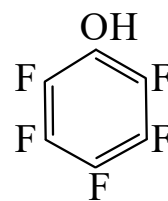




>>Entry Name: Pentafluorophenol, 9CI



CAS Registry Number: 771-61-9

Molecular Formula: C₆HF₅O

Molecular Weight: 184.065

Accurate Mass: 183.994755

Percentage Composition: C 39.15%; H 0.55%; F 51.61%; O 8.69%

Physical Description: Cryst.

Melting Point: Mp 38.5-39.5°

Boiling Point: Bp 142-144°

Hazard & Toxicity: LD₅₀ (rat, scu) 322 mg/kg

Aldrich: 10379-9

Fluka: 76740

Sigma: P3271

Supelco: 44-2745

>>Derivative: Formyl

Synonym(s): Pentafluorophenyl formate. Pentafluorophenol formate, 9CI

CAS Registry Number: 111333-97-2

Molecular Formula: C₇HF₅O₂

Molecular Weight: 212.076

Accurate Mass: 211.98967

Percentage Composition: C 39.64%; H 0.48%; F 44.79%; O 15.09%

Use/Importance: Formylating reagent

Physical Description: Oil

Density: d²⁰ 1.67

Other Data: Slowly dec. at r.t.

>>Derivative: Trifluoroacetyl

CAS Registry Number: 14533-84-7

Molecular Formula: C₈F₈O₂

Molecular Weight: 280.074

Accurate Mass: 279.977054

Percentage Composition: C 34.31%; F 54.27%; O 11.43%

Physical Description: Liq.

Melting Point: Mp 3.1-3.6°

Boiling Point: Bp 122-123°

Refractive Index: n_D²⁰ 1.3680

Aldrich: 37707-4

Fluka: 91725

>>Derivative: Benzoyl

Molecular Formula: C₁₃H₅F₅O₂

Molecular Weight: 288.173

Accurate Mass: 288.02097

Percentage Composition: C 54.18%; H 1.75%; F 32.96%; O 11.10%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 70.5-71.5°