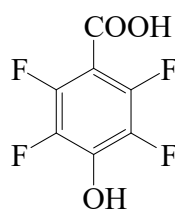




>>Entry Name: 2,3,5,6-Tetrafluoro-4-hydroxybenzoic acid, 9CI



CAS Registry Number: 652-34-6

Related CAS Registry Numbers(s): 27375-81-1

Molecular Formula: C₇H₂F₄O₃

Molecular Weight: 210.085

Accurate Mass: 209.994007

Percentage Composition: C 40.02%; H 0.96%; F 36.17%; O 22.85%

Melting Point: Mp 155-157°

pKa Value: pK_{a1} 2.27; pK_{a2} 5.17 (25°, H₂O)

>>Derivative: Monohydrate

CAS Registry Number: 143201-17-6

Melting Point: Mp 104-107°

>>Derivative: Et ester

CAS Registry Number: 123270-98-4

Molecular Formula: C₉H₆F₄O₃

Molecular Weight: 238.138

Accurate Mass: 238.025307

Percentage Composition: C 45.39%; H 2.54%; F 31.91%; O 20.16%

Physical Description: Cryst.

Melting Point: Mp 108-110°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-2,3,5,6-tetrafluorophenol

CAS Registry Number: 19161-30-9

Molecular Formula: C₇HF₄NO

Molecular Weight: 191.085

Accurate Mass: 190.999426

Percentage Composition: C 44.00%; H 0.53%; F 39.77%; N 7.33%; O 8.37%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 128-129° (124°)

>>Derivative: Nitrile, *O*-benzoyl

CAS Registry Number: 31469-88-2

Molecular Formula: C₁₄H₅F₄NO₂

Molecular Weight: 295.193

Accurate Mass: 295.025641

Percentage Composition: C 56.96%; H 1.71%; F 25.74%; N 4.74%; O 10.84%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 113-114°

>>Derivative: Me ether

Synonym(s): 2,3,5,6-Tetrafluoro-4-methoxybenzoic acid

CAS Registry Number: 3153-01-3

Molecular Formula: C₈H₄F₄O₃

Molecular Weight: 224.111

Accurate Mass: 224.009657

Percentage Composition: C 42.88%; H 1.80%; F 33.91%; O 21.42%

Physical Description: Cryst.

Melting Point: Mp 122-123°