



>>Entry Name: 4-Hydroxy-3,5-dimethylbenzoic acid

Synonym(s): 4-Hydroxymesitylenic acid. 4-Hydroxy-*sym-m*-xylic acid. 2,6-Xylenol-4-carboxylic acid

CAS Registry Number: 4919-37-3

Molecular Formula: C₉H₁₀O₃

Molecular Weight: 166.176

Accurate Mass: 166.062995

Percentage Composition: C 65.05%; H 6.07%; O 28.88%

Physical Description: Cryst. (H₂O or C₆H₆)

Melting Point: Mp 226-227.5°

Rare Chemicals Library: S43836-7

>>Derivative: Me ester

CAS Registry Number: 34137-14-9

Molecular Formula: C₁₀H₁₂O₃

Molecular Weight: 180.203

Accurate Mass: 180.078645

Percentage Composition: C 66.65%; H 6.71%; O 26.64%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 130°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-2,6-dimethylphenol

CAS Registry Number: 4198-90-7

Molecular Formula: C₉H₉NO

Molecular Weight: 147.176

Accurate Mass: 147.068414

Percentage Composition: C 73.45%; H 6.16%; N 9.52%; O 10.87%

Physical Description: Cryst. (petrol)

Melting Point: Mp 126°

pKa Value: p*K*_{a1} 8.19 (25°)

>>Derivative: Ac

Molecular Formula: C₁₁H₁₂O₄

Molecular Weight: 208.213

Accurate Mass: 208.07356

Percentage Composition: C 63.45%; H 5.81%; O 30.74%

Physical Description: Cryst. (petrol)

Melting Point: Mp 98°

>>Derivative: Me ether

Synonym(s): 4-Methoxy-3,5-dimethylbenzoic acid. 3,5-Dimethyl-*p*-anisic acid

CAS Registry Number: 21553-46-8

Molecular Formula: C₁₀H₁₂O₃

Molecular Weight: 180.203

Accurate Mass: 180.078645

Percentage Composition: C 66.65%; H 6.71%; O 26.64%

Biological Source: Component of Fan Xie Ye

Physical Description: Needles (petrol)

Melting Point: Mp 196-198°