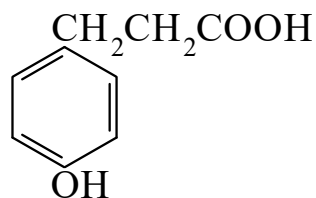




>>>Entry Name: 3-(4-Hydroxyphenyl)propanoic acid

Synonym(s): 4-Hydroxybenzenepropanoic acid, 9Cl. 3-(*p*-Hydroxyphenyl)propionic acid, 8Cl. Dihydro-*p*-coumaric acid. *p*-Hydroxyhydrocinnamic acid. Phloretinic acid. HPPA. Phloretic acid



CAS Registry Number: 501-97-3

Molecular Formula: C₉H₁₀O₃

Molecular Weight: 166.176

Accurate Mass: 166.062995

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

Biological Source: Constit. of urine. Isol. from sulfite liquors, prod. by *Clostridium butyricum*. Isol. from heartwood of *Haplormosia monophylla* (Leguminosae). A prod. of tyrosine metab.; conc. in urine increases in patients with gastrointestinal diseases

Use/Importance: Fluorescent substrate for the detn. of peroxidase

Physical Description: Prisms (Et₂O)

Melting Point: Mp 129-130°

pKa Value: pK_a 4.76 (25°)

Aldrich: H5240-6

Fluka: 56190

Sigma: H6386

>>>Derivative: Me ester

CAS Registry Number: 5597-50-2

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. (Et₂O/petrol)

Melting Point: Mp 40-41°

Boiling Point: Bp₁₇ 186-187°

Aldrich: 36091-0

>>>Derivative: Et ester

Molecular Formula: C₁₁H₁₄O₃

Molecular Weight: 194.23

Accurate Mass: 194.094295

Percentage Composition: C 68.02%; H 7.26%; O 24.71%

Melting Point: Mp 45°

Boiling Point: Bp₁₈ 193°

>>>Derivative: 4-Methylpentyl ester

Molecular Formula: C₁₅H₂₂O₃

Molecular Weight: 250.337

Accurate Mass: 250.156895

Percentage Composition: C 71.97%; H 8.86%; O 19.17%

Biological Source: Constit. of *Cheirolophus mauritanicus*

Physical Description: Gum

>>>Derivative: Tridecyl ester

CAS Registry Number: 232262-50-9

Molecular Formula: C₂₂H₃₆O₃

Molecular Weight: 348.525

Accurate Mass: 348.266445

Percentage Composition: C 75.82%; H 10.41%; O 13.77%

Biological Source: Constit. of *Piper longum*