



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

Synonym(s): 3-Hydroxybenzenepropanoic acid, 9Cl. 3-(*m*-Hydroxyphenyl)propionic acid, 8Cl. 3-Hydroxyhydrocinnamic acid

CAS Registry Number: 621-54-5

Molecular Formula: C₉H₁₀O₃

Molecular Weight: 166.176

Accurate Mass: 166.062995

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

Physical Description: Needles (C₆H₆/petrol)

Melting Point: Mp 111°

Hazard & Toxicity: LD₅₀ (mus, orl) >2g/kg

>>Derivative: Me ether

Synonym(s): 3-(3-Methoxyphenyl)propanoic acid. 3-Methoxyhydrocinnamic acid

CAS Registry Number: 10516-71-9

Molecular Formula: C₁₀H₁₂O₃

Molecular Weight: 180.203

Accurate Mass: 180.078645

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

Physical Description: Needles

Melting Point: Mp 51°

pKa Value: pK_a 4.65 (25°)

Aldrich: 34976-3

>>Derivative: Me ether, Me 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 29-30°

Boiling Point: Bp₈ 140-141°

>>Derivative: Me ether, Et ester

Molecular Formula: C₁₂H₁₆O₃

Molecular Weight: 208.257

Accurate Mass: 208.109945

Percentage Composition: C 69.21%; H 7.74%; O 23.05%

Boiling Point: Bp₁₇ 183-184°

>>Derivative: Me ether, chloride

Molecular Formula: C₁₀H₁₁ClO₂

Molecular Weight: 198.648

Accurate Mass: 198.044757

Percentage Composition: C 60.46%; H 5.58%; Cl 17.85%; O 16.11%

Physical Description: Yellow oil

Boiling Point: Bp₂₂ 165°

>>Derivative: Me ether, amide

Molecular Formula: C₁₀H₁₃NO₂

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Melting Point: Mp 55-56°

Boiling Point: Bp₉ 218-219°

References: