



Molecular Formula: C₉H₁₁NO₂
Molecular Weight: 165.191
Accurate Mass: 165.078979
Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%
Physical Description: Prisms
Melting Point: Mp 58-59°

>>Derivative: Ac

Molecular Formula: C₁₁H₁₂O₄
Molecular Weight: 208.213
Accurate Mass: 208.07356
Percentage Composition: C 63.45%; H 5.81%; O 30.74%
Melting Point: Mp 93.5-95.5°

>>Derivative: Me ether

Synonym(s): 3-(4-Methoxyphenyl)propanoic acid

CAS Registry Number: 1929-29-9
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. (EtOH or H₂O)
Melting Point: Mp 104-105°
Boiling Point: Bp₁₅ 192-194°
pKa Value: pK_{a1} 4.71 (25°)
Aldrich: M2352-7
Fluka: 65235
Rare Chemicals Library: S11854-0

>>Derivative: Me ether, Me ester

CAS Registry Number: 15823-04-8
Molecular Formula: C₁₁H₁₄O₃
Molecular Weight: 194.23
Accurate Mass: 194.094295
Percentage Composition: C 68.02%; H 7.26%; O 24.71%
Physical Description: Plates (H₂O)
Melting Point: Mp 38°
Boiling Point: Bp 278°. Bp₁ 120°

>>Derivative: Me ether, amide

CAS Registry Number: 25413-27-8
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%
Physical Description: Prisms (EtOH)
Melting Point: Mp 125-126°
Rare Chemicals Library: S85009-8

>>Derivative: Me ether, nitrile

CAS Registry Number: 22442-48-4
Molecular Formula: C₁₀H₁₁NO
Molecular Weight: 161.203
Accurate Mass: 161.084064
Percentage Composition: C 74.51%; H 6.88%; N 8.69%; O 9.93%
Boiling Point: Bp 290-300°. Bp₁₅ 167°

References: