



>>Entry Name: **3-(4-Methylphenyl)-2-propenoic acid**, 9CI
Synonym(s): *p*-Methylcinnamic acid, 8CI. 3-*p*-Tolylacrylic acid

CAS Registry Number: 1866-39-3
Related CAS Registry Numbers(s): 18254-00-7 20511-20-0 28446-70-0 35121-92-7 70625-62-6

Molecular Formula: C₁₀H₁₀O₂
Molecular Weight: 162.188
Accurate Mass: 162.06808
Percentage Composition: C 74.06%; H 6.21%; O 19.73%

Aldrich: M3580-0

>>Variant: (*E*)-form

CAS Registry Number: 940-61-4
Molecular Formula: C₁₀H₁₀O₂
Molecular Weight: 162.188
Accurate Mass: 162.06808
Percentage Composition: C 74.06%; H 6.21%; O 19.73%
Physical Description: Needles (EtOH or C₆H₆)
Melting Point: Mp 198-199°
pKa Value: pK_a 4.56

>>Derivative: Me ester

CAS Registry Number: 20754-20-5
Molecular Formula: C₁₁H₁₂O₂
Molecular Weight: 176.215
Accurate Mass: 176.08373
Percentage Composition: C 74.98%; H 6.86%; O 18.16%
Physical Description: Cryst. (EtOH aq.)
Melting Point: Mp 57-58°
Boiling Point: Bp₃₂ 164-165°

>>Derivative: Et ester

CAS Registry Number: 24393-49-5
Molecular Formula: C₁₂H₁₄O₂
Molecular Weight: 190.241
Accurate Mass: 190.09938
Percentage Composition: C 75.76%; H 7.42%; O 16.82%
Boiling Point: Bp 278°. Bp₁₇ 158-159°

>>Derivative: Nitrile

CAS Registry Number: 35121-93-8
Molecular Formula: C₁₀H₉N
Molecular Weight: 143.188
Accurate Mass: 143.073499
Percentage Composition: C 83.88%; H 6.34%; N 9.78%
Melting Point: Mp 69-80°

>>Derivative: Amide

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%
Physical Description: Plates (CHCl₃)
Melting Point: Mp 189-190°

>>Variant: (*Z*)-form