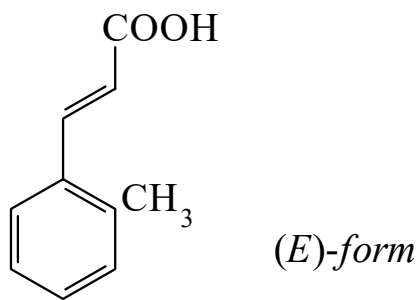




>>Entry Name: 3-(2-Methylphenyl)-2-propenoic acid, 9CI

Synonym(s): *o*-Methylcinnamic acid, 8CI. 3-*o*-Tolylacrylic acid



CAS Registry Number: 2373-76-4

Related CAS Registry Numbers(s): 16366-23-7 83716-65-8

Molecular Formula: C₁₀H₁₀O₂

Molecular Weight: 162.188

Accurate Mass: 162.06808

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

pKa Value: p*K*_a 4.5

Aldrich: 43310-1

>>Variant: (*E*)-form

CAS Registry Number: 939-57-1

Molecular Formula: C₁₀H₁₀O₂

Molecular Weight: 162.188

Accurate Mass: 162.06808

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

Physical Description: Cryst. (EtOH or C₆H₆)

Melting Point: Mp 175-176°

>>Derivative: Et ester

CAS Registry Number: 24393-48-4

Molecular Formula: C₁₂H₁₄O₂

Molecular Weight: 190.241

Accurate Mass: 190.09938

Percentage Composition: C 75.76%; H 7.42%; O 16.82%

Physical Description: Oil

Boiling Point: Bp_{2.2} 114-117°. Bp_{1.2} 148°

>>Derivative: Amide

Synonym(s): 3-(2-Methylphenyl)-2-propenamide. U 77863. Antibiotic U 77863

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%

Biological Source: Prod. by *Streptomyces griseoluteus*

Biological Use/Importance: Exhibits antitumour props.

Physical Description: Cryst. (MeOH)

Melting Point: Mp 151-153°

UV: [neutral] λ_{max} 208 (ε 17300); 220 (ε 14900); 225 (sh) (ε 12000); 276 (ε 16500) (MeOH) (Derep) [neutral] λ_{max} 208 (ε 17320); 220 (ε 14900); 276 (ε 16540) (MeOH) (Berdy)

>>Variant: (*Z*)-form

CAS Registry Number: 41397-71-1

Molecular Formula: C₁₀H₁₀O₂

Molecular Weight: 162.188

Accurate Mass: 162.06808

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

Melting Point: Mp 91-92° (89-90°)

References: