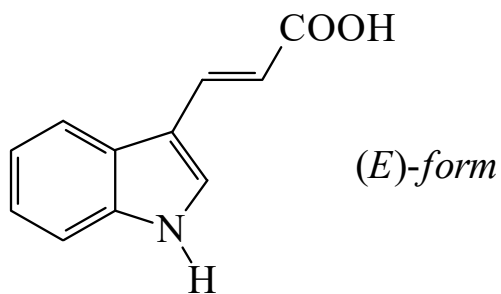




>>Entry Name: 3-(1*H*-Indol-3-yl)-2-propenoic acid

Synonym(s): 1*H*-Indole-3-propenoic acid. 3-(3-Indolyl)acrylic acid



CAS Registry Number: 1204-06-4

Molecular Formula: C₁₁H₉NO₂

Molecular Weight: 187.198

Accurate Mass: 187.063329

Percentage Composition: C 70.58%; H 4.85%; N 7.48%; O 17.09%

Biological Source: Major auxin from roots of *Lens culinaris* (Leguminosae)

Hazard & Toxicity: Exp. carcinogenic data

Fluka: 57290

Sigma: I1625

>>Variant: (*E*)-form

CAS Registry Number: 29953-71-7

Molecular Formula: C₁₁H₉NO₂

Molecular Weight: 187.198

Accurate Mass: 187.063329

Percentage Composition: C 70.58%; H 4.85%; N 7.48%; O 17.09%

Biological Source: Alkaloid from the red alga *Chondria* sp.

Physical Description: Red-brown cryst. (H₂O or AcOH)

Melting Point: Mp 195-196°

Aldrich: I-380-7

>>Derivative: Me ester

Molecular Formula: C₁₂H₁₁NO₂

Molecular Weight: 201.224

Accurate Mass: 201.078979

Percentage Composition: C 71.63%; H 5.51%; N 6.96%; O 15.90%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 153-154°

>>Derivative: Me ester, *N*-Ac

Molecular Formula: C₁₄H₁₃NO₃

Molecular Weight: 243.262

Accurate Mass: 243.089544

Percentage Composition: C 69.12%; H 5.39%; N 5.76%; O 19.73%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 179-180°

>>Derivative: Amide

Synonym(s): 3-(1*H*-Indol-3-yl)-2-propenamide. 3-(3-Indolyl)acrylamide

Molecular Formula: C₁₁H₁₀N₂O

Molecular Weight: 186.213

Accurate Mass: 186.079313

Percentage Composition: C 70.95%; H 5.41%; N 15.04%; O 8.59%

Biological Source: Alkaloid from *Chondria atropurpurea*

Physical Description: Amber cryst. (Me₂CO)

Melting Point: Mp 212.8-214.2°

UV: [neutral] λ_{max} 226 (log ε 1.49); 275 (log ε 1.25); 322 (log ε 1.55) (MeOH) [neutral] λ_{max} 226 (); 275 (); 322 () (MeOH) (Berdy)