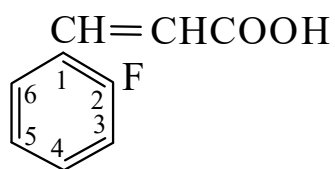




>>Entry Name: 3-(2-Fluorophenyl)-2-propenoic acid, 9CI

Synonym(s): *o*-Fluorocinnamic acid



CAS Registry Number: 451-69-4

Molecular Formula: C₉H₇FO₂

Molecular Weight: 166.151

Accurate Mass: 166.043008

Percentage Composition: C 65.06%; H 4.25%; F 11.43%; O 19.26%

Physical Description: Needles (H₂O)

Melting Point: Mp 175°

pKa Value: pK_{a1} 4.28 (25°)

Aldrich: 22271-2

>>Derivative: Et ester

CAS Registry Number: 348-13-0

Molecular Formula: C₁₁H₁₁FO₂

Molecular Weight: 194.205

Accurate Mass: 194.074308

Percentage Composition: C 68.03%; H 5.71%; F 9.78%; O 16.48%

Boiling Point: Bp₁₁ 140-141°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1044C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 175C, (*ir*)

Willstaedt, H., *Ber.*, 1931, **64**, 2688, (*synth*)

Japan. Pat., 1975, 75 70 589; *CA*, **84**, 72652