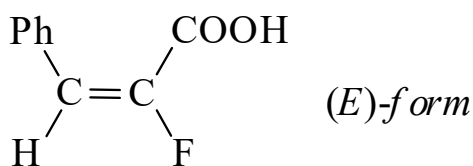




>>Entry Name: 2-Fluoro-3-phenyl-2-propenoic acid, 9CI

Synonym(s): α -Fluorocinnamic acid



CAS Registry Number: 350-90-3

Related CAS Registry Numbers(s): 350-99-2 370-07-0 56695-78-4 56695-79-5

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%

Aldrich: 16384-8

Sigma: F1253

>>Variant: (E)-form

CAS Registry Number: 20397-60-8

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: Cryst. (EtOH aq.)

>>Derivative: Et ester

CAS Registry Number: 20397-58-4

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: Bp_{0.6} 93°

>>Variant: (Z)-form

CAS Registry Number: 20397-61-9

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%

Melting Point: Mp 157.6°

Boiling Point: Bp 290°

pK_a Value: pK_a 2.9 (25°)

>>Derivative: Et ester

CAS Registry Number: 20397-59-5

Molecular Formula: C₁₁H₁₁FO₂

Molecular Weight: 194.205

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

Boiling Point: Bp_{1.5} 82°

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 175A, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1044B, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1321D, (*ir*)
Swarts, F., *Bull. Soc. Chim. Fr.*, 1919, **25**, 325
Elhrich, E. *et al.*, *Bull. Soc. Chim. Fr.*, 1973, 1277-1280, (*synth*)
Normant, J.F. *et al.*, *Synthesis*, 1975, 122-125, (*synth*)
Elkik, E. *et al.*, *Bull. Soc. Chim. Fr.*, 1986, 423-428, (*cmr*, *pmr*, *F-19 nmr*, *derivs*)
Kayser, M.M. *et al.*, *Can. J. Chem.*, 1997, **75**, 1315-1321, (*Et ester*, *synth*, *pmr*)
Kanasaki, T. *et al.*, *J.O.C.*, 1998, **63**, 7525-7528, (*Me ester*, *synth*, *pmr*, *cmr*)
Ishihara, T. *et al.*, *Tet. Lett.*, 1998, **39**, 4865-4868, (*synth*)