>>**Entry Name: 3-(Pentafluorophenyl)-2-propenoic acid,** 9CI
Synonym(s): 2,3,4,5,6-Pentafluorocinnamic acid

CAS Registry Number: 719-60-8
Related CAS Registry Numbers(s): 79168-76-6
$(C_6F_5)CH=CHCOOH$

Molecular Formula: $C_9H_3F_5O_2$
Molecular Weight: 238.113
Accurate Mass: 238.00532
Percentage Composition: C 45.40%; H 1.27%; F 39.89%; O 13.44%

Aldrich: 29052-1
Sigma: P1044

>>**Variant:** (*E*)-form

CAS Registry Number: 34234-46-3
Molecular Formula: $C_9H_3F_5O_2$
Molecular Weight: 238.113
Accurate Mass: 238.00532
Percentage Composition: C 45.40%; H 1.27%; F 39.89%; O 13.44%
Physical Description: Cryst. (EtOH/petrol)
Melting Point: Mp 154-156°

>>**Derivative:** Me ester

CAS Registry Number: 39720-45-1
Molecular Formula: $C_{10}H_5F_5O_2$
Molecular Weight: 252.14
Accurate Mass: 252.02097
Percentage Composition: C 47.64%; H 2.00%; F 37.67%; O 12.69%
Boiling Point: Bp_2 70°

>>**Derivative:** Et ester

CAS Registry Number: 83004-28-8
Molecular Formula: $C_{11}H_7F_5O_2$
Molecular Weight: 266.167
Accurate Mass: 266.03662
Percentage Composition: C 49.64%; H 2.65%; F 35.69%; O 12.02%
Boiling Point: Bp_2 78°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1061A, *(nmr)*
Barbour, A.K. *et al.*, *J.C.S.*, 1961, 808, *(synth)*
Filler, R. *et al.*, *J.O.C.*, 1975, **40**, 935, *(synth, uv)*
Shen, Y. *et al.*, *Synth. Commun.*, 1991, **21**, 1403, *(synth, ir, pmr, F-19 nmr, ms, esters)*