



>>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

$(\text{C}_6\text{F}_5)\text{CH}=\text{CHCOOH}$

Molecular Formula: $\text{C}_9\text{H}_3\text{F}_5\text{O}_2$

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: $\text{C}_9\text{H}_3\text{F}_5\text{O}_2$

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: $\text{C}_{10}\text{H}_5\text{F}_5\text{O}_2$

Molecular Weight: 252.14

Accurate Mass: 252.02097

Percentage Composition: C 47.64%; H 2.00%; F 37.67%; O 12.69%

Boiling Point: Bp₂ 70°

>>Derivative: Et ester

CAS Registry Number: 83004-28-8

Molecular Formula: $\text{C}_{11}\text{H}_7\text{F}_5\text{O}_2$

Molecular Weight: 266.167

Accurate Mass: 266.03662

Percentage Composition: C 49.64%; H 2.65%; F 35.69%; O 12.02%

Boiling Point: Bp₂ 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*)