



>>Entry Name: (Difluoromethyl)phosphonic acid, 9CI

CAS Registry Number: 74963-39-6

Related CAS Registry Numbers(s): 681-80-1 83567-74-2 94993-99-4 110624-90-3
F2CHP(O)(OH)2

Molecular Formula: CH3F2O3P

Molecular Weight: 132.003

Accurate Mass: 131.978788

Percentage Composition: C 9.10%; H 2.29%; F 28.78%; O 36.36%; P 23.46%

>>Derivative: Bis(cyclohexylammonium) salt

CAS Registry Number: 110624-94-7

Physical Description: Solid

Melting Point: Mp 193-195°

>>Derivative: Di-Et ester

Synonym(s): Diethyl (difluoromethyl)phosphonate

CAS Registry Number: 1478-53-1

Molecular Formula: C5H11F2O3P

Molecular Weight: 188.111

Accurate Mass: 188.041388

Percentage Composition: C 31.93%; H 5.89%; F 20.20%; O 25.52%; P 16.47%

Use/Importance: Wittig-Horner reagent for the synth. of 1,1-difluoroalkenes

Physical Description: Liq.

Boiling Point: Bp₁₂ 85.5-86.5°. Bp_{1.5} 62°

Aldrich: 41141-8

>>Derivative: Di-2-propenyl ester

Synonym(s): Di-2-propenyl (difluoromethyl)phosphonate. Diallyl (difluoromethyl)phosphonate

Molecular Formula: C7H11F2O3P

Molecular Weight: 212.133

Accurate Mass: 212.041388

Percentage Composition: C 39.63%; H 5.23%; F 17.91%; O 22.63%; P 14.60%

Source/Synthesis: Reagent for synth. of (1,1-difluoroalkyl)phosphonic acids

Physical Description: Liq.

Boiling Point: Bp_{0.2} 60°

>>Derivative: Dichloride

CAS Registry Number: 1554-44-5

Molecular Formula: CHCl2F2OP

Molecular Weight: 168.894

Accurate Mass: 167.911012

Percentage Composition: C 7.11%; H 0.60%; Cl 41.98%; F 22.50%; O 9.47%; P 18.34%

Physical Description: Liq.

Boiling Point: Bp 128-133°. Bp₅₀ 50-52°

References:

- Soborovskii, L.Z. *et al.*, *Zh. Obshch. Khim.*, 1959, **29**, 1144; *J. Gen. Chem. USSR (Engl. Transl.)*, 1959, **29**, 1115, (*synth*)
McKenna, C.E. *et al.*, *J.O.C.*, 1981, **46**, 4536, (*synth, pmr, F-19 nmr, P-31 nmr*)
Obayashi, M. *et al.*, *Tet. Lett.*, 1982, **23**, 2323, (*synth, use*)
Hall, C.R. *et al.*, *J.C.S. Perkin 1*, 1985, 233, (*esters*)
Blackburn, G.M. *et al.*, *J.C.S. Perkin 1*, 1987, 181
Bergstrom, D.E. *et al.*, *J.O.C.*, 1988, **53**, 3953, (*di-Et ester, dichloride, synth*)
Berkowitz, D.B. *et al.*, *J.O.C.*, 1995, **60**, 7047, (*dialkyl ester*)