# Dimethyl {1-[2-(2-fluorophenoxy)acetoxy]-ethyl}phosphonate

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Key indicators

Single-crystal X-ray study
T = 272 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.109
Data-to-parameter ratio = 18.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The crystal structure of the title compound, $C_{12}H_{16}FO_6P$, is stabilized by intermolecular C—H···O hydrogen bonds.

Comment

α-Hydroxyalkylphosphonate derivatives are of considerable interest as potential biologically active compounds or pharmaceuticals (He, 2003). We have synthesized a new α-hydroxyethylphosphonate derivative, (I). Here, we report its structure (Fig. 1).

(I)
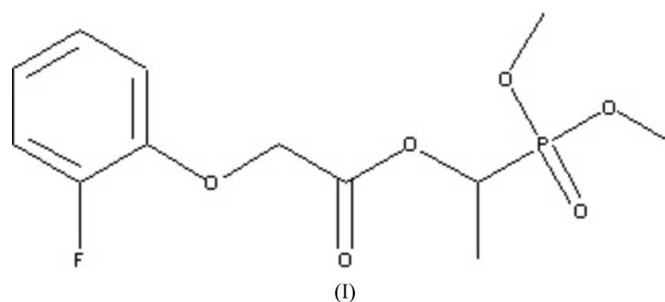
Selected bond distances and angles are listed in Table 1. The molecules are connected by intermolecular C—H···O hydrogen bonds (Table 2), forming a layer parallel to the (010) plane (Fig. 2).

Experimental

The title compound was synthesized by the reaction of dimethyl 1-hydroxyethylphosphonate and 2-fluorophenoxyacetyl chloride according to a literature procedure (He *et al.*, 1998). Crystals suitable
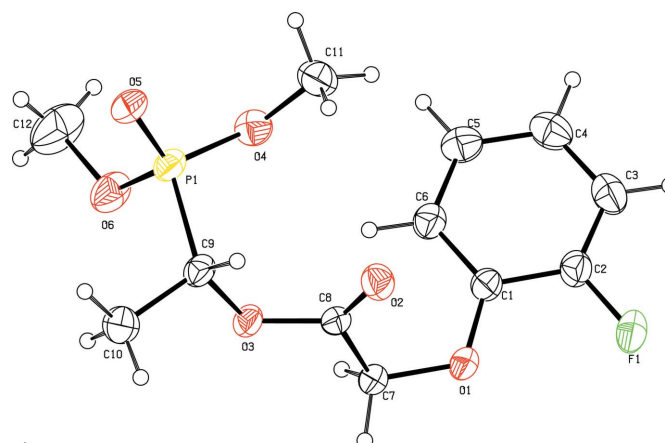
Figure 1
The structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

organic papers

for X-ray diffraction were obtained by slow evaporation of a petroleum ether/dichloromethane (4:1 v/v) solution at 293 K.

Crystal data

$C_{12}H_{16}FO_6P$
$M_r = 306.22$
Monoclinic, $P2_1/c$
$a = 8.7321 (8)$ Å
$b = 18.3099 (16)$ Å
$c = 9.2048 (8)$ Å
$\beta = 99.448 (2)°$
$V = 1451.7 (2)$ Å^3
$Z = 4$

$D_x = 1.401$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4456 reflections
$\theta = 2.2–28.2°$
$\mu = 0.22$ mm^{-1}
$T = 272 (2)$ K
Block, colorless
$0.30 \times 0.30 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
9060 measured reflections
3314 independent reflections

2851 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 27.5°$
$h = -11 \rightarrow 10$
$k = -23 \rightarrow 23$
$l = -11 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.109$
$S = 1.03$
3314 reflections
184 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0569P)^2 + 0.3545P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.3704 (19)	C9—P1	1.8110 (15)
C7—O1	1.4178 (18)	C11—O4	1.447 (2)
C8—O2	1.1927 (17)	O4—P1	1.5682 (13)
C8—O3	1.3454 (17)	O5—P1	1.4649 (11)
C9—O3	1.4573 (16)	O6—P1	1.5688 (13)
O1—C1—C6	126.52 (14)	C8—O3—C9	117.31 (11)
O3—C8—C7	108.99 (12)	O5—P1—O6	116.09 (7)
C1—O1—C7	116.99 (12)	O4—P1—O6	102.03 (8)

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C3—H3⋯O5^i	0.93	2.51	3.416 (2)	165
C7—H7A⋯O5^{ii}	0.97	2.39	3.2793 (19)	152
C9—H9⋯O2	0.98	2.33	2.7241 (19)	103

Symmetry codes: (i) $x + 1, y, z + 1$; (ii) $x + 1, y, z$.

Figure 2
The packing of (I), showing C—H⋯O hydrogen bonds as dashed lines. Suffixes a and b correspond to symmetry codes (i) and (ii), respectively, in Table 2.

H atoms were placed at calculated positions (C—H = 0.93–0.98 Å) and refined as riding, with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

References

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