Methyl (4-acetylphenoxy)acetate

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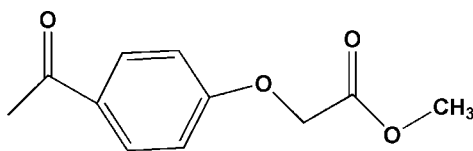Correspondence e-mail: liuyy21@yahoo.com.cn

The molecule of the title compound, $C_{11}H_{12}O_4$, is essentially planar. The OCH_2COOCH_3 group is extended away from the aromatic ring, with an O—C—C—O torsion angle of 173.9 (1)°.

Related literature

For related literature, see: Gonzàlez-Duarte *et al.* (1996); Ping *et al.* (2007); Ríos-Moreno *et al.* (2003).

Experimental

Crystal data

$C_{11}H_{12}O_4$	V = 2075.0 (2) Å^3
M_r = 208.21	Z = 8
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
a = 24.690 (1) Å	μ = 0.10 mm^{-1}
b = 7.5580 (6) Å	T = 273 (2) K
c = 11.1280 (9) Å	0.40 × 0.30 × 0.25 mm
β = 92.230 (1)°	

Data collection

Bruker APEX CCD area-detector diffractometer	6117 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2421 independent reflections
T_{min} = 0.970, T_{max} = 0.980	1872 reflections with $I > 2\sigma(I)$
	R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047	136 parameters
$wR(F^2)$ = 0.144	H-atom parameters constrained
S = 1.06	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
2421 reflections	$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

References

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supplementary materials

Methyl (4-acetylphenoxy)acetate

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Comment

As shown in Fig. 1, the title compound (I), in which the OCH_2COOCH_3 group is extended away from the aromatic ring with an O—C—C—O torsion angle of 173.9 (1)°, is essentially planar ignoring all hydrogen atoms.

The C10—O3 and C10—O4 bond lengths are 1.193 (2) and 1.327 (2) Å, respectively, and the O3—C10—O4 angle is 125.2 (1)°. The C10—O3 distance is shorter than that found in other similar coordinated ester molecules (Gonzàlez-Duarte *et al.*, 1996; Ríos-Moreno *et al.*, 2003), while the C10—O4 distance is shorter than that found in another similar ester (Ping *et al.*, 2007).

Experimental

A mixture of ethyl *p*-hydroxybenzoate (8.3 g, 50 mmol) and NaOH (2.0 g, 50 mmol) in DMSO (10 ml) was stirred at 333 K for 1 h, and then the methyl chloroacetate (5.4 g, 50 mmol) was added. The mixture was cooled to room temperature after stirring at 333 K for 2 h, then poured into 200 ml of water and a white solid formed immediately. The obtained precipitate (0.20 g) was dissolved in 15 ml me thanol, and colorless single crystals of (I) were obtained after several days at room temperature.

Refinement

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with d(C—H) = 0.93 Å, $U_{iso} = 1.2U_{eq}(C)$ for aromatic, 0.97 Å, $U_{iso} = 1.5U_{eq}(C)$ for CH_2 atoms and 0.96 Å, $U_{iso} = 1.5U_{eq}(C)$ for CH_3 atoms.

Figures
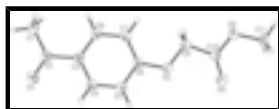

Fig. 1. View of the structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

Methyl 4-acetylphenoxyacetate

Crystal data

$C_{11}H_{12}O_4$	$F_{000} = 880$
$M_r = 208.21$	$D_x = 1.333$ Mg m^{-3}
Monoclinic, $C2/c$	Melting point: not measured K
Hall symbol: -C 2yc	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å

$a = 24.6900$ (10) Å

$b = 7.5580$ (6) Å

$c = 11.1280$ (9) Å

$\beta = 92.2300$ (10)º

$V = 2075.0$ (2) Å^3

$Z = 8$

Cell parameters from 2421 reflections

$\theta = 3.3$–28.2º

$\mu = 0.10$ mm^{-1}

$T = 273$ (2) K

Block, colorless

$0.40 \times 0.30 \times 0.25$ mm

Data collection

Bruker APEX CCD area-detector diffractometer	2421 independent reflections
Radiation source: fine-focus sealed tube	1872 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 273(2)$ K	$\theta_{max} = 28.2$º
ω scans	$\theta_{min} = 3.3$º
Absorption correction: empirical (using intensity measurements) (SADABS; Sheldrick, 1996)	$h = -32 \rightarrow 20$
$T_{min} = 0.970$, $T_{max} = 0.980$	$k = -9 \rightarrow 9$
6117 measured reflections	$l = -14 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.144$	$w = 1/[\sigma^2(F_o^2) + (0.081P)^2 + 0.3709P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = <0.001$
2421 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
136 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of F^2 > 2sigma(F^2) is used only for calculating R-factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.23473 (6)	0.5091 (3)	0.57792 (15)	0.0612 (4)
H1A	0.2014	0.5370	0.6155	0.092*
H1B	0.2285	0.4154	0.5208	0.092*
H1C	0.2477	0.6119	0.5373	0.092*
C2	0.27612 (5)	0.45135 (19)	0.67172 (12)	0.0462 (3)
C3	0.33143 (5)	0.40001 (17)	0.63545 (11)	0.0402 (3)
C4	0.36934 (5)	0.34295 (19)	0.72408 (12)	0.0446 (3)
H4	0.3596	0.3384	0.8039	0.054*
C5	0.42082 (5)	0.29360 (19)	0.69471 (12)	0.0465 (3)
H5	0.4456	0.2557	0.7544	0.056*
C6	0.43570 (5)	0.30052 (18)	0.57537 (12)	0.0428 (3)
C7	0.39911 (5)	0.3578 (2)	0.48646 (12)	0.0482 (3)
H7	0.4091	0.3632	0.4068	0.058*
C8	0.34732 (5)	0.40702 (19)	0.51710 (12)	0.0458 (3)
H8	0.3227	0.4455	0.4573	0.055*
C9	0.50411 (5)	0.2400 (2)	0.43547 (12)	0.0478 (3)
H9A	0.5012	0.3564	0.3991	0.057*
H9B	0.4814	0.1589	0.3886	0.057*
C10	0.56212 (5)	0.17801 (18)	0.43853 (12)	0.0448 (3)
C11	0.63673 (7)	0.1337 (3)	0.31544 (18)	0.0683 (5)
H11A	0.6459	0.1441	0.2327	0.102*
H11B	0.6412	0.0131	0.3410	0.102*
H11C	0.6601	0.2085	0.3640	0.102*
O1	0.26456 (5)	0.4471 (2)	0.77717 (10)	0.0760 (4)
O2	0.48748 (4)	0.24604 (15)	0.55592 (9)	0.0551 (3)
O3	0.58735 (4)	0.12804 (18)	0.52558 (10)	0.0651 (3)
O4	0.58085 (4)	0.18728 (16)	0.32852 (10)	0.0598 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0409 (7)	0.0861 (12)	0.0568 (9)	0.0101 (7)	0.0047 (6)	0.0061 (8)
C2	0.0401 (7)	0.0560 (8)	0.0428 (7)	−0.0026 (6)	0.0065 (5)	−0.0018 (6)
C3	0.0369 (6)	0.0444 (7)	0.0394 (7)	−0.0024 (5)	0.0032 (5)	−0.0017 (5)
C4	0.0442 (7)	0.0570 (8)	0.0328 (6)	−0.0010 (6)	0.0033 (5)	−0.0023 (5)
C5	0.0417 (7)	0.0619 (8)	0.0356 (7)	0.0034 (6)	−0.0034 (5)	−0.0007 (6)
C6	0.0348 (6)	0.0548 (8)	0.0389 (7)	0.0008 (5)	0.0016 (5)	−0.0031 (5)
C7	0.0426 (7)	0.0674 (9)	0.0346 (7)	0.0035 (6)	0.0039 (5)	0.0027 (6)
C8	0.0389 (7)	0.0598 (8)	0.0384 (7)	0.0036 (6)	−0.0001 (5)	0.0046 (6)
C9	0.0378 (7)	0.0668 (9)	0.0389 (7)	0.0043 (6)	0.0027 (5)	−0.0006 (6)
C10	0.0397 (7)	0.0509 (7)	0.0440 (7)	−0.0004 (5)	0.0023 (5)	−0.0050 (6)
C11	0.0483 (8)	0.0781 (11)	0.0800 (12)	0.0131 (7)	0.0222 (8)	0.0037 (9)
O1	0.0512 (7)	0.1315 (12)	0.0459 (6)	0.0128 (7)	0.0118 (5)	0.0011 (6)
O2	0.0374 (5)	0.0899 (8)	0.0381 (5)	0.0112 (5)	0.0021 (4)	−0.0023 (5)

| O3 | 0.0523 (6) | 0.0943 (9) | 0.0485 (6) | 0.0169 (6) | −0.0022 (5) | −0.0011 (5) |
| O4 | 0.0454 (6) | 0.0848 (8) | 0.0501 (6) | 0.0140 (5) | 0.0117 (4) | 0.0036 (5) |

Geometric parameters (Å, °)

C1—C2	1.497 (2)	C7—C8	1.3871 (18)
C1—H1A	0.9600	C7—H7	0.9300
C1—H1B	0.9600	C8—H8	0.9300
C1—H1C	0.9600	C9—O2	1.418 (2)
C2—O1	1.219 (2)	C9—C10	1.5062 (19)
C2—C3	1.4903 (18)	C9—H9A	0.9700
C3—C8	1.3898 (18)	C9—H9B	0.9700
C3—C4	1.4010 (18)	C10—O3	1.193 (2)
C4—C5	1.3761 (18)	C10—O4	1.327 (2)
C4—H4	0.9300	C11—O4	1.4505 (17)
C5—C6	1.3926 (18)	C11—H11A	0.9600
C5—H5	0.9300	C11—H11B	0.9600
C6—O2	1.368 (2)	C11—H11C	0.9600
C6—C7	1.3830 (18)		
C2—C1—H1A	109.5	C6—C7—H7	120.3
C2—C1—H1B	109.5	C8—C7—H7	120.3
H1A—C1—H1B	109.5	C7—C8—C3	121.31 (12)
C2—C1—H1C	109.5	C7—C8—H8	119.3
H1A—C1—H1C	109.5	C3—C8—H8	119.3
H1B—C1—H1C	109.5	O2—C9—C10	107.38 (11)
O1—C2—C3	120.35 (13)	O2—C9—H9A	110.2
O1—C2—C1	119.99 (13)	C10—C9—H9A	110.2
C3—C2—C1	119.66 (12)	O2—C9—H9B	110.2
C8—C3—C4	118.25 (12)	C10—C9—H9B	110.2
C8—C3—C2	122.82 (12)	H9A—C9—H9B	108.5
C4—C3—C2	118.92 (12)	O3—C10—O4	125.2 (1)
C5—C4—C3	120.95 (12)	O3—C10—C9	125.67 (13)
C5—C4—H4	119.5	O4—C10—C9	109.14 (11)
C3—C4—H4	119.5	O4—C11—H11A	109.5
C4—C5—C6	119.78 (12)	O4—C11—H11B	109.5
C4—C5—H5	120.1	H11A—C11—H11B	109.5
C6—C5—H5	120.1	O4—C11—H11C	109.5
O2—C6—C7	124.70 (12)	H11A—C11—H11C	109.5
O2—C6—C5	114.98 (11)	H11B—C11—H11C	109.5
C7—C6—C5	120.31 (12)	C6—O2—C9	117.77 (10)
C6—C7—C8	119.40 (12)	C10—O4—C11	116.4 (1)
O1—C2—C3—C8	−178.17 (14)	C6—C7—C8—C3	0.0 (2)
C1—C2—C3—C8	1.6 (2)	C4—C3—C8—C7	0.5 (2)
O1—C2—C3—C4	1.5 (2)	C2—C3—C8—C7	−179.83 (13)
C1—C2—C3—C4	−178.75 (13)	O2—C9—C10—O3	6.3 (2)
C8—C3—C4—C5	−0.6 (2)	O2—C9—C10—O4	−173.91 (12)
C2—C3—C4—C5	179.75 (13)	C7—C6—O2—C9	−3.0 (2)
C3—C4—C5—C6	0.1 (2)	C5—C6—O2—C9	176.37 (13)
C4—C5—C6—O2	−179.04 (12)	C10—C9—O2—C6	179.56 (11)

C4—C5—C6—C7	0.4 (2)	O3—C10—O4—C11	−0.8 (2)
O2—C6—C7—C8	178.92 (13)	C9—C10—O4—C11	179.40 (13)
C5—C6—C7—C8	−0.5 (2)		

Fig. 1