Acta Crystallographica Section E
**Structure Reports**
**Online**
ISSN 1600-5368

# 2-(4-Chlorophenyl)-2-oxoethyl 4-methylbenzoate

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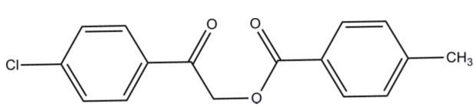
Received 14 October 2011; accepted 16 October 2011

Key indicators: single-crystal X-ray study; $T$ = 297 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.046; $wR$ factor = 0.144; data-to-parameter ratio = 22.4.

In the title compound, $C_{16}H_{13}ClO_3$, the dihedral angle between the benzene rings is 80.74 (8)°. In the crystal, C—H···O hydrogen bonds link the molecules to form $C$(11) chains propagating in [010].

## Related literature

For a related structure and background references to phenacyl benzoates, see: Fun *et al.* (2011).




## Experimental

*Crystal data*

$C_{16}H_{13}ClO_3$
$M_r$ = 288.71
Monoclinic, $P2_1/c$
$a$ = 5.9132 (4) Å
$b$ = 8.5044 (6) Å
$c$ = 27.8767 (18) Å
$\beta$ = 95.880 (1)°
$V$ = 1394.49 (16) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.28 mm$^{-1}$
$T$ = 297 K
0.51 × 0.30 × 0.06 mm

*Data collection*

Bruker SMART APEXII DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.871, $T_{max}$ = 0.983
21275 measured reflections
4070 independent reflections
2628 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.144
$S$ = 1.05
4070 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C16—H16$C$···O1$^{i}$ | 0.96 | 2.46 | 3.383 (2) | 162 |

Symmetry code: (i) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PLATON* (Spek, 2009).

HKF and WSL thank Universiti Sains Malaysia (USM) for the Research University Grant (No. 1001/PFIZIK/811160). WSL also thanks the Malaysian government and USM for the award of the post of Research Officer under the Research University Grant (No. 1001/PFIZIK/811160). AMI thanks Professor Sandeep Sanchethi, Director of the National Institute of Technology-Karnataka, India for providing the research facilities. AMI also thanks the Board for Research in Nuclear Sciences, Department of Atomic Energy, Government of India for the 'Young Scientist' award. MNS thanks the Department of Information Technology, Government of India for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6454).

## References

Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fun, H.-K., Loh, W.-S., Garudachari, B., Isloor, A. M. & Satyanarayana, M. N. (2011). *Acta Cryst.* E**67**, o2854.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

‡ Thomson Reuters ResearcherID: A-3561-2009.
§ Thomson Reuters ResearcherID: C-7581-2009.

# supplementary materials

*Acta Cryst.* (2011). E**67**, o3030 [ **doi:10.1107/S1600536811042851** ]

## 2-(4-Chlorophenyl)-2-oxoethyl 4-methylbenzoate

**H.-K. Fun, W.-S. Loh, B. Garudachari, A. M. Isloor and M. N. Satyanarayana**

### Comment

As part of our ongoing studies of phenacyl benzoates (Fun *et al.*, 2011), we now report the synthesis and sturcture of the title compound, (I).

In the title compound (Fig. 1), the dihedral angle formed between the chloro-substituted (C1–C6) and the methyl-substituted (C10–C15) benzene rings is 80.74 (8)°. Bond lengths and angles are within the normal ranges and are comparable to a related structure (Fun *et al.*, 2011).

In the crystal (Fig. 2), intermolecular C16—H16C···O1 hydrogen bonds (Table 1) link the molecules to form chains along the *b* axis.

### Experimental

A mixture of 4-methylbenzoic acid (1.0 g, 0.0073 mol), potassium carbonate (1.10 g, 0.0080 mol) and 2-bromo-1-(4-chlorophenyl)ethanone (1.70 g, 0.0073 mol) in dimethylformamide (10 ml) was stirred at room temperature for 2 h. On cooling, colourless needle-shaped crystals of the title compound began to separate out. They were collected by filtration and recrystallized from ethanol to yield colourless plates of (I). Yield: 1.95 g, 92.8%. *M. p*: 405–406 K.

### Refinement

All H atoms were positioned geometrically and refined with a riding model with $U_{iso}$(H) = 1.2 or 1.5 $U_{eq}$(C) [C–H = 0.93 or 0.97 Å]. A rotating group model was applied to the methyl group.

### Figures

Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

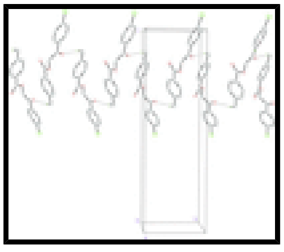


Fig. 2. The crystal packing of the title compound, viewed along the showing the *a* axis. H atoms not involved in the intermolecular interactions (dashed lines) have been omitted for clarity.

## 2-(4-Chlorophenyl)-2-oxoethyl 4-methylbenzoate

### *Crystal data*

| | |
|---|---|
| $C_{16}H_{13}ClO_3$ | $F(000) = 600$ |
| $M_r = 288.71$ | $D_x = 1.375$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 4428 reflections |
| $a = 5.9132$ (4) Å | $\theta = 2.8$–28.1° |
| $b = 8.5044$ (6) Å | $\mu = 0.28$ mm$^{-1}$ |
| $c = 27.8767$ (18) Å | $T = 297$ K |
| $\beta = 95.880$ (1)° | Plate, colourless |
| $V = 1394.49$ (16) Å$^3$ | 0.51 × 0.30 × 0.06 mm |
| $Z = 4$ | |

### *Data collection*

| | |
|---|---|
| Bruker SMART APEXII DUO CCD diffractometer | 4070 independent reflections |
| Radiation source: fine-focus sealed tube | 2628 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.027$ |
| φ and ω scans | $\theta_{max} = 30.1°$, $\theta_{min} = 1.5°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | $h = -8 \rightarrow 8$ |
| $T_{min} = 0.871$, $T_{max} = 0.983$ | $k = -11 \rightarrow 12$ |
| 21275 measured reflections | $l = -39 \rightarrow 39$ |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.046$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.144$ | H-atom parameters constrained |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.3124P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 4070 reflections | $(\Delta/\sigma)_{max} = 0.002$ |
| 182 parameters | $\Delta\rho_{max} = 0.20$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.42$ e Å$^{-3}$ |

### *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 $F^2 > \sigma(F^2)$ 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 1.34410 (11) | 0.75388 (9) | 1.047675 (19) | 0.0935 (2) |
| O1 | 0.5306 (2) | 0.69016 (17) | 0.86404 (5) | 0.0739 (4) |
| O2 | 0.6246 (2) | 0.50027 (17) | 0.79276 (4) | 0.0612 (3) |
| O3 | 0.3791 (2) | 0.35541 (15) | 0.83027 (4) | 0.0643 (3) |
| C1 | 0.8059 (3) | 0.7539 (2) | 0.94970 (7) | 0.0569 (4) |
| H1A | 0.6646 | 0.8027 | 0.9453 | 0.068* |
| C2 | 0.9496 (4) | 0.7851 (2) | 0.99053 (7) | 0.0646 (5) |
| H2A | 0.9056 | 0.8539 | 1.0138 | 0.078* |
| C3 | 1.1586 (3) | 0.7138 (2) | 0.99658 (6) | 0.0589 (4) |
| C4 | 1.2267 (3) | 0.6099 (2) | 0.96302 (6) | 0.0598 (4) |
| H4A | 1.3684 | 0.5617 | 0.9678 | 0.072* |
| C5 | 1.0808 (3) | 0.5784 (2) | 0.92215 (6) | 0.0530 (4) |
| H5A | 1.1248 | 0.5083 | 0.8992 | 0.064* |
| C6 | 0.8693 (3) | 0.65035 (18) | 0.91501 (5) | 0.0462 (3) |
| C7 | 0.7093 (3) | 0.62133 (19) | 0.87099 (6) | 0.0487 (4) |
| C8 | 0.7785 (3) | 0.5032 (2) | 0.83558 (6) | 0.0579 (4) |
| H8A | 0.9298 | 0.5283 | 0.8273 | 0.070* |
| H8B | 0.7842 | 0.3997 | 0.8503 | 0.070* |
| C9 | 0.4256 (3) | 0.42441 (19) | 0.79494 (6) | 0.0484 (4) |
| C10 | 0.2774 (3) | 0.43770 (17) | 0.74889 (5) | 0.0438 (3) |
| C11 | 0.3350 (3) | 0.53418 (19) | 0.71169 (6) | 0.0496 (4) |
| H11A | 0.4730 | 0.5876 | 0.7146 | 0.060* |
| C12 | 0.1863 (3) | 0.55014 (19) | 0.67042 (6) | 0.0523 (4) |
| H12A | 0.2264 | 0.6144 | 0.6456 | 0.063* |
| C13 | −0.0210 (3) | 0.47287 (18) | 0.66499 (5) | 0.0482 (4) |
| C14 | −0.0734 (3) | 0.3726 (2) | 0.70156 (6) | 0.0531 (4) |
| H14A | −0.2093 | 0.3166 | 0.6982 | 0.064* |
| C15 | 0.0749 (3) | 0.3551 (2) | 0.74308 (6) | 0.0505 (4) |
| H15A | 0.0379 | 0.2873 | 0.7672 | 0.061* |
| C16 | −0.1878 (3) | 0.5006 (2) | 0.62043 (6) | 0.0604 (4) |
| H16A | −0.1102 | 0.4892 | 0.5920 | 0.091* |
| H16B | −0.2492 | 0.6049 | 0.6215 | 0.091* |
| H16C | −0.3089 | 0.4252 | 0.6197 | 0.091* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| Cl1 | 0.0873 (4) | 0.1316 (6) | 0.0578 (3) | −0.0190 (4) | −0.0114 (3) | −0.0225 (3) |
| O1 | 0.0601 (8) | 0.0737 (8) | 0.0831 (9) | 0.0200 (7) | −0.0156 (7) | −0.0148 (7) |
| O2 | 0.0487 (6) | 0.0890 (9) | 0.0452 (6) | −0.0116 (6) | 0.0008 (5) | −0.0060 (6) |
| O3 | 0.0746 (8) | 0.0656 (8) | 0.0513 (7) | −0.0104 (7) | −0.0006 (6) | 0.0087 (6) |
| C1 | 0.0517 (9) | 0.0576 (10) | 0.0617 (10) | 0.0007 (8) | 0.0071 (8) | −0.0088 (8) |
| C2 | 0.0714 (12) | 0.0683 (11) | 0.0555 (10) | −0.0103 (10) | 0.0130 (9) | −0.0163 (8) |
| C3 | 0.0615 (10) | 0.0705 (11) | 0.0438 (8) | −0.0165 (9) | 0.0011 (7) | −0.0034 (8) |
| C4 | 0.0510 (9) | 0.0736 (11) | 0.0526 (9) | 0.0014 (8) | −0.0044 (7) | −0.0015 (8) |
| C5 | 0.0518 (9) | 0.0582 (9) | 0.0480 (8) | 0.0033 (7) | 0.0011 (7) | −0.0065 (7) |
| C6 | 0.0466 (8) | 0.0462 (8) | 0.0457 (8) | −0.0043 (6) | 0.0039 (6) | −0.0001 (6) |
| C7 | 0.0452 (8) | 0.0482 (8) | 0.0518 (8) | −0.0021 (7) | −0.0002 (7) | 0.0017 (7) |
| C8 | 0.0470 (9) | 0.0747 (11) | 0.0503 (9) | 0.0005 (8) | −0.0042 (7) | −0.0102 (8) |
| C9 | 0.0497 (8) | 0.0485 (8) | 0.0469 (8) | 0.0006 (7) | 0.0046 (7) | −0.0075 (7) |
| C10 | 0.0455 (8) | 0.0443 (7) | 0.0418 (7) | −0.0007 (6) | 0.0059 (6) | −0.0054 (6) |
| C11 | 0.0483 (8) | 0.0488 (8) | 0.0522 (8) | −0.0082 (7) | 0.0071 (7) | 0.0001 (7) |
| C12 | 0.0617 (10) | 0.0492 (8) | 0.0467 (8) | −0.0037 (7) | 0.0081 (7) | 0.0046 (7) |
| C13 | 0.0532 (9) | 0.0478 (8) | 0.0431 (8) | 0.0039 (7) | 0.0030 (6) | −0.0083 (6) |
| C14 | 0.0483 (8) | 0.0598 (10) | 0.0508 (8) | −0.0109 (7) | 0.0040 (7) | −0.0052 (7) |
| C15 | 0.0518 (9) | 0.0555 (9) | 0.0449 (8) | −0.0097 (7) | 0.0082 (7) | 0.0004 (7) |
| C16 | 0.0638 (11) | 0.0631 (10) | 0.0524 (9) | 0.0048 (9) | −0.0030 (8) | −0.0047 (8) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cl1—C3 | 1.7400 (17) | C8—H8A | 0.9700 |
| O1—C7 | 1.2062 (19) | C8—H8B | 0.9700 |
| O2—C9 | 1.349 (2) | C9—C10 | 1.483 (2) |
| O2—C8 | 1.4250 (18) | C10—C15 | 1.383 (2) |
| O3—C9 | 1.203 (2) | C10—C11 | 1.392 (2) |
| C1—C2 | 1.375 (2) | C11—C12 | 1.381 (2) |
| C1—C6 | 1.387 (2) | C11—H11A | 0.9300 |
| C1—H1A | 0.9300 | C12—C13 | 1.385 (2) |
| C2—C3 | 1.371 (3) | C12—H12A | 0.9300 |
| C2—H2A | 0.9300 | C13—C14 | 1.388 (2) |
| C3—C4 | 1.377 (3) | C13—C16 | 1.523 (2) |
| C4—C5 | 1.383 (2) | C14—C15 | 1.387 (2) |
| C4—H4A | 0.9300 | C14—H14A | 0.9300 |
| C5—C6 | 1.388 (2) | C15—H15A | 0.9300 |
| C5—H5A | 0.9300 | C16—H16A | 0.9600 |
| C6—C7 | 1.491 (2) | C16—H16B | 0.9600 |
| C7—C8 | 1.495 (2) | C16—H16C | 0.9600 |
| C9—O2—C8 | 117.12 (13) | O3—C9—O2 | 122.98 (15) |
| C2—C1—C6 | 120.75 (17) | O3—C9—C10 | 125.56 (15) |
| C2—C1—H1A | 119.6 | O2—C9—C10 | 111.46 (14) |
| C6—C1—H1A | 119.6 | C15—C10—C11 | 119.15 (14) |
| C3—C2—C1 | 119.28 (17) | C15—C10—C9 | 119.38 (14) |
| C3—C2—H2A | 120.4 | C11—C10—C9 | 121.45 (14) |
| C1—C2—H2A | 120.4 | C12—C11—C10 | 119.66 (15) |
| C2—C3—C4 | 121.52 (16) | C12—C11—H11A | 120.2 |
| C2—C3—Cl1 | 119.91 (15) | C10—C11—H11A | 120.2 |

| | | | |
|---|---|---|---|
| C4—C3—Cl1 | 118.57 (15) | C11—C12—C13 | 121.67 (15) |
| C3—C4—C5 | 118.90 (17) | C11—C12—H12A | 119.2 |
| C3—C4—H4A | 120.5 | C13—C12—H12A | 119.2 |
| C5—C4—H4A | 120.5 | C12—C13—C14 | 118.22 (14) |
| C4—C5—C6 | 120.60 (16) | C12—C13—C16 | 120.48 (15) |
| C4—C5—H5A | 119.7 | C14—C13—C16 | 121.28 (15) |
| C6—C5—H5A | 119.7 | C15—C14—C13 | 120.59 (15) |
| C1—C6—C5 | 118.94 (15) | C15—C14—H14A | 119.7 |
| C1—C6—C7 | 118.97 (15) | C13—C14—H14A | 119.7 |
| C5—C6—C7 | 122.08 (14) | C10—C15—C14 | 120.61 (15) |
| O1—C7—C6 | 121.57 (15) | C10—C15—H15A | 119.7 |
| O1—C7—C8 | 120.98 (15) | C14—C15—H15A | 119.7 |
| C6—C7—C8 | 117.46 (13) | C13—C16—H16A | 109.5 |
| O2—C8—C7 | 111.72 (14) | C13—C16—H16B | 109.5 |
| O2—C8—H8A | 109.3 | H16A—C16—H16B | 109.5 |
| C7—C8—H8A | 109.3 | C13—C16—H16C | 109.5 |
| O2—C8—H8B | 109.3 | H16A—C16—H16C | 109.5 |
| C7—C8—H8B | 109.3 | H16B—C16—H16C | 109.5 |
| H8A—C8—H8B | 107.9 | | |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | 0.6 (3) | C8—O2—C9—O3 | −3.1 (2) |
| C1—C2—C3—C4 | −0.9 (3) | C8—O2—C9—C10 | 176.99 (14) |
| C1—C2—C3—Cl1 | 179.20 (14) | O3—C9—C10—C15 | −5.7 (2) |
| C2—C3—C4—C5 | 0.6 (3) | O2—C9—C10—C15 | 174.20 (14) |
| Cl1—C3—C4—C5 | −179.55 (14) | O3—C9—C10—C11 | 172.90 (16) |
| C3—C4—C5—C6 | 0.1 (3) | O2—C9—C10—C11 | −7.2 (2) |
| C2—C1—C6—C5 | 0.0 (3) | C15—C10—C11—C12 | 2.2 (2) |
| C2—C1—C6—C7 | −179.28 (16) | C9—C10—C11—C12 | −176.38 (15) |
| C4—C5—C6—C1 | −0.4 (3) | C10—C11—C12—C13 | 0.3 (3) |
| C4—C5—C6—C7 | 178.91 (16) | C11—C12—C13—C14 | −2.6 (2) |
| C1—C6—C7—O1 | 2.9 (3) | C11—C12—C13—C16 | 176.20 (15) |
| C5—C6—C7—O1 | −176.38 (18) | C12—C13—C14—C15 | 2.3 (2) |
| C1—C6—C7—C8 | −177.07 (16) | C16—C13—C14—C15 | −176.49 (15) |
| C5—C6—C7—C8 | 3.6 (2) | C11—C10—C15—C14 | −2.5 (2) |
| C9—O2—C8—C7 | −77.7 (2) | C9—C10—C15—C14 | 176.13 (15) |
| O1—C7—C8—O2 | 7.0 (3) | C13—C14—C15—C10 | 0.2 (3) |
| C6—C7—C8—O2 | −173.03 (14) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C16—H16C···O1$^{i}$ | 0.96 | 2.46 | 3.383 (2) | 162 |

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+3/2.

**Fig. 1**

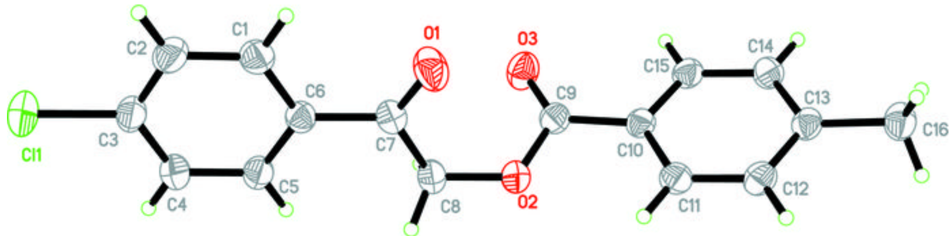


**Fig. 2**