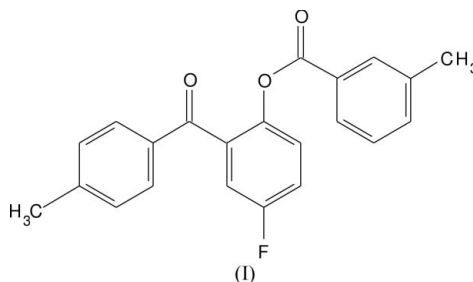


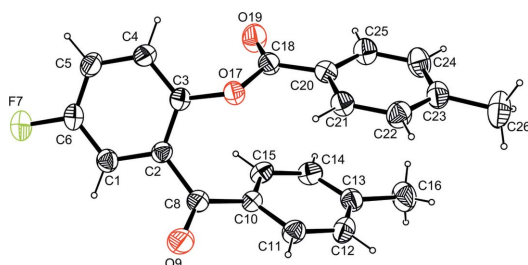
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Key indicators

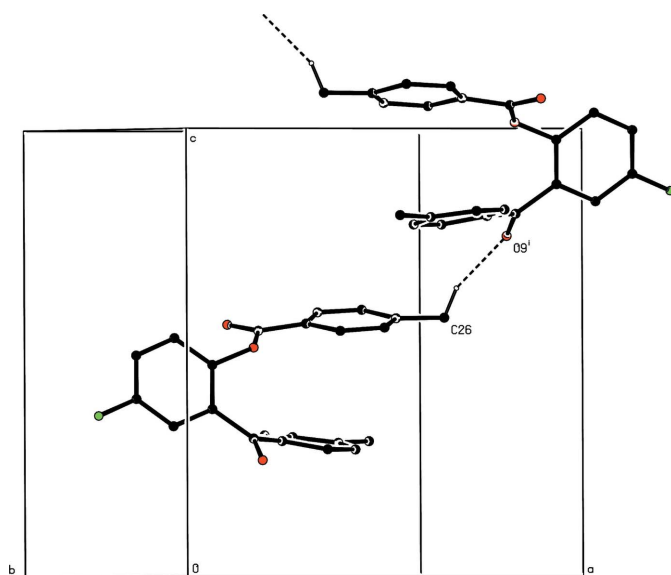
Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(C-C) = 0.005$ Å
 R factor = 0.038
 wR factor = 0.120
Data-to-parameter ratio = 6.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.[5-Fluoro-2-(4-methylbenzoyloxy)phenyl]-
(4-methylphenyl)methanoneIn the title compound, $C_{22}H_{17}FO_3$, there are weak inter-
molecular $C-H \cdots O$ hydrogen bonds resulting in the forma-
tion of a polymeric chain.Received 6 November 2006
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Comment

Benzophenones are a class of compounds obtained from
natural products (Henry *et al.*, 1999) or by synthetic methods
(Karrer *et al.*, 2000). The great interest in these substances is
fundamentally due to their diverse biological and chemical
properties. Synthetic benzophenones, such as 2-amino-
benzophenone (Liou *et al.*, 2002) and dihydroxy-4-methoxy-
benzophenone (Nakagawa & Suzuki, 2002), have proven to be
antimitotic and anticancer agents, respectively. Recently, *para*-
methoxy substituted benzophenones were evaluated as p38a
inhibitors with high efficiency and selectivity (Revesz *et al.*,
2004). Amino- and methoxy-substituted benzophenones are
reported to be potent cytotoxic agents against a panel of
human cancer cell lines including multidrug resistant cell lines.
Benzophenones exhibit anti-inflammatory (Khanum *et al.*,
2004), antimicrobial, anti-allergic, anti-asthmatic and anti-
anaphylactic activities. They are also used as core steroid
sulfatase (STS) inhibitors with IC₅₀ values between 5 and
7 μ M. These compounds are evaluated as inhibitors of HIV
reverse transcriptase (RT) and the growth of HIV in MT-4
cells.The title compound, (I), has three benzene rings which are
linked *via* carbonyl and ester groups (Fig. 1). The dihedral
angle between the two aromatic rings linked by the keto
carbonyl group is $64.27(17)^\circ$, while that about the benzene
rings linked by the ester group is $58.51(17)^\circ$. These values
differ significantly from the corresponding values of $65.99(12)^\circ$
and $69.33(12)^\circ$, and $68.95(9)^\circ$ and $54.98(9)^\circ$ reported for
2-[(4-methylbenzoyloxy)-5-methylphenyl]phenylmethanone
(Naveen *et al.*, 2006) and 2-benzoyloxy-5-methylbenzophe-
none (Sieroń *et al.*, 2004) respectively. The conformation of
the attachment of the benzoyl and benzoate rings to the
central benzene ring can also be characterized by torsion
angles $C1-C2-C8-C10$ and $C2-C3-O17-C18$ of

**Figure 1**

The molecular structure, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

**Figure 2**

A partial packing diagram, showing the weak C—H···O hydrogen bonding interactions. H atoms not involved in hydrogen bonds have been omitted for clarity. Hydrogen bonds are represented as dashed lines. [Symmetry code: (i) $1 - x, -y, \frac{1}{2} + z$

138.3 (3) and 123.5 (3)°, respectively. The carbonyl groups at C8 and C18 are oriented in $-$ synclinal and $+$ synperiplanar conformations, respectively, as indicated by the torsion angle values of -41.3 (5) and 9.9 (5)° for C1—C2—C8—O9 and C3—O17—C18—O19 respectively. The molecules are linked by intermolecular C—H···O interactions between the methylphenyl ring and the carbonyl group of the keto group to form a polymeric chain (Table 1, Fig. 2).

Experimental

To a well stirred ice cold solution of (2-hydroxy-5-fluorophenyl)-4-methylphenylmethanone (3 g, 0.014 mol), in 10% sodium hydroxide (20 ml), 4-methylbenzoyl chloride (1.96 g, 0.01 mol) was added dropwise and stirring was continued for about 20 min. The mixture was made alkaline by adding 10% sodium hydroxide. A white solid separated, which was filtered off and washed with water. On recrystallization from ethanol, a pale-green solid was obtained with a yield of 81%. M.p. 365 K. Analysis calculated for C₂₂H₁₇FO₃: C 75.85, H 4.92, F 5.45%; found: C 75.84, H 4.91, F 5.44%.

Crystal data

C₂₂H₁₇FO₃
M_r = 348.36
 Orthorhombic, *Pca*2₁
a = 13.519 (10) Å
b = 9.902 (9) Å
c = 13.319 (17) Å
V = 1783 (3) Å³

Z = 4
D_x = 1.298 Mg m⁻³
 Mo *K*α radiation
 μ = 0.09 mm⁻¹
T = 295 (2) K
 Block, pale green
 0.25 × 0.20 × 0.20 mm

Data collection

MacScience DIPLabo 32001
 diffractometer
 ω scans
 Absorption correction: none
 2860 measured reflections

1625 independent reflections
 1457 reflections with $I > 2\sigma(I)$
*R*_{int} = 0.018
 θ_{\max} = 25.0°

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.038
wR(*F*²) = 0.120
S = 1.11
 1625 reflections
 237 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0703P)^2 + 0.2402P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.11 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.14 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C26—H26B···O9 ⁱ	0.96	2.49	3.355 (8)	149

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

H atoms were placed at idealized positions and allowed to ride on their parent atoms with C—H distances in the range 0.93–0.96 Å; *U*_{iso}(H) values were set equal to *xU*_{eq}(carrier atom), where *x* = 1.5 for methyl H atoms and 1.2 for all other H atoms. In the absence of significant anomalous scattering, Friedel pairs were merged.

Data collection: *XPRESS* (MacScience, 2002); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-III* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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References

- Burnett, M. N. & Johnson, C. K. (1996). *ORTEP-III*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Henry, G. E., Jacobs, H., Carrington, C. M. S., Mclean, S. & Reynolds, W. F. (1999). *Tetrahedron*, **55**, 1581–1596.
 Karrer, F., Meier, H. & Pascual, A. (2000). *J. Fluorine Chem.* **103**, 81–84.
 Khanum, S. A., Venu, T. D., Shashikanth, S. & Firdouse, A. (2004). *Bioorg. Med. Chem. Lett.* **14**, 5351–5355.
 Liou, G. P., Chang, C. W., Song, J. S., Yang, Y. N., Yeh, C. F., Tseng, H. Y., Lo, Y. K., Chang, Y. L., Chang, C. M. & Hsieh, H. P. (2002). *J. Med. Chem.* **45**, 2556–2562.
 MacScience (2002). *XPRESS*. MacScience Co. Ltd, Yokohama, Japan.
 Nakagawa, Y. & Suzuki, T. (2002). *Chem. Biol. Interact.* **139**, 115–128.
 Naveen, S., Venu, T. D., Shashikanth, S., Sridhar, M. A. & Shashidhara Prasad, J. (2006). *Anal. Sci.* **22**, x155–x156.

- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
- Revesz, L., Blum, F. E., Di Padova, E. T., Buhl, R., Feifel, H., Gram, P., Hiestand, U., Manning, A. & Rucklin, G. (2004). *Bioorg. Med. Chem. Lett.* **14**, 3601–3605.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sieroń, L., Shashikanth, S., Yathirajan, H. S., Venu, T. D., Nagaraj, B., Nagaraja, P. & Khanum, S. A. (2004). *Acta Cryst. E* **60**, o1889–o1891.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.