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[5-Fluoro-2-(4-methylbenzoyloxy)phenyl]-(4-methylphenyl)methanone

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.038
wR factor = 0.120
Data-to-parameter ratio = 6.9

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

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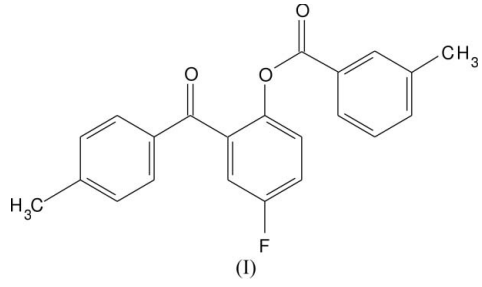
In the title compound, $C_{22}H_{17}FO_3$, there are weak intermolecular C—H···O hydrogen bonds resulting in the formation of a polymeric chain.

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-aminobenzophenone (Liou *et al.*, 2002) and dihydroxy-4-methoxybenzophenone (Nakagawa & Suzuki, 2002), have proven to be antimitotic and anticancer agents, respectively. Recently, *para*-methoxy substituted benzophenones were evaluated as p38*a* 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-asthamatic 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.



(I)

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)°, while that about the benzene rings linked by the ester group is 58.51 (17)°. These values differ significantly from the corresponding values of 65.99 (12) and 69.33 (12)°, and 68.95 (9) and 54.98 (9)° reported for 2-[(4-methylbenzoyloxy)-5-methylphenyl]phenylmethanone (Naveen *et al.*, 2006) and 2-benzoyloxy-5-methylbenzophenone (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

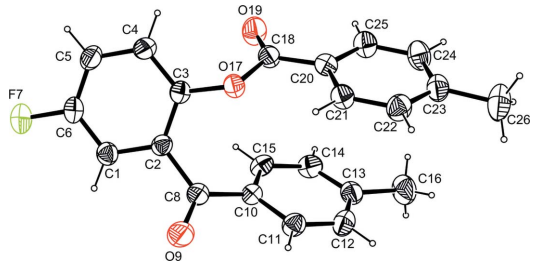


Figure 1
The molecular structure, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

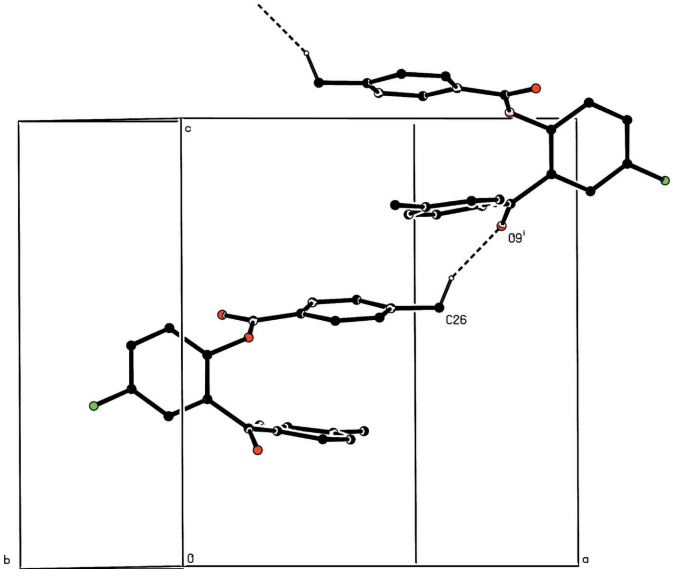


Figure 2
A partial packing diagram, showing the weak C—H···O hydrogen bonding interactions. H atoms not involved in hydrogen bonds have been omitted for clarity. Hydrogen bonds are represented as dashed lines. [Symmetry code: (i) $1-x, -y, \frac{1}{2}+z$

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 $C_{22}H_{17}FO_3$: C 75.85, H 4.92, F 5.45%; found: C 75.84, H 4.91, F 5.44%.

Crystal data

$C_{22}H_{17}FO_3$
$M_r = 348.36$
Orthorhombic, $Pca2_1$
$a = 13.519\ (10)$ Å
$b = 9.902\ (9)$ Å
$c = 13.319\ (17)$ Å
$V = 1783\ (3)$ Å^3
$Z = 4$
$D_x = 1.298$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ 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 $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.120$
$S = 1.11$
1625 reflections
237 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0703P)^2 + 0.2402P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
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: *ORTEPIII* (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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