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Methyl 7-(4-chlorobenzoyloxy)-1,3-benzodioxole-5-carboxylate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.119
Data-to-parameter ratio = 12.6

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

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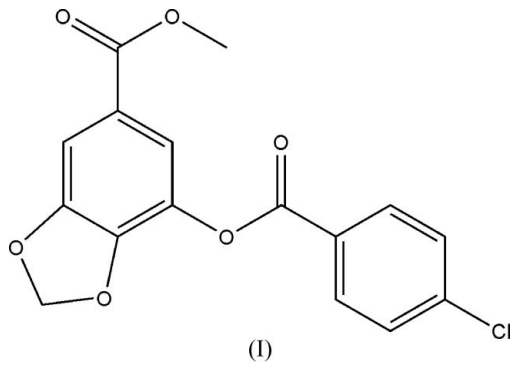
In the title compound, $C_{16}H_{11}ClO_6$, the dihedral angle between the two benzene rings is 86.9 (3)°.

Comment

Because of their interesting properties, not only as pharmacologically active compounds, but also as chiral reagents, natural biaryls and their derivatives constitute attractive synthetic goals. The key step in such syntheses is almost always the coupling of the two aromatic halves of the molecule. The title compound, (I) (Fig. 1), is a representative of the building blocks of biaryls.



(I)

In the molecule of (I), the mean planes of the C3–C9 (*A*) and C11–C16 (*B*) benzene rings are inclined to each other at an angle of 86.9 (3)°. The mean planes of rings *A* and *B* make dihedral angles of 2.5 (3) and 84.5 (3)°, respectively, with the mean plane of the C5/C6/C7/O3/O4 ring.

Experimental

The title compound was synthesized by the reaction of 4-chlorobenzoic acid and methyl 7-hydroxybenzo[*d*][1,3]dioxole-5-carboxylate in the presence of dicyclohexylcarbodiimide (DCC) and 4-(dimethylamino)pyridine (DMAP) (Bringmann *et al.*, 2002). Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a petroleum ether–ethyl acetate (10:1 *v*/*v*) mixture (m.p. 387–388 K).

Crystal data

$C_{16}H_{11}ClO_6$
M_r = 334.70
Monoclinic, $P2_1/n$
a = 12.240 (5) Å
b = 6.618 (3) Å
c = 18.471 (8) Å
β = 95.879 (7)°
V = 1488.3 (11) Å^3
Z = 4
D_x = 1.494 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 294 (2) K
Block, colourless
0.24 × 0.20 × 0.14 mm

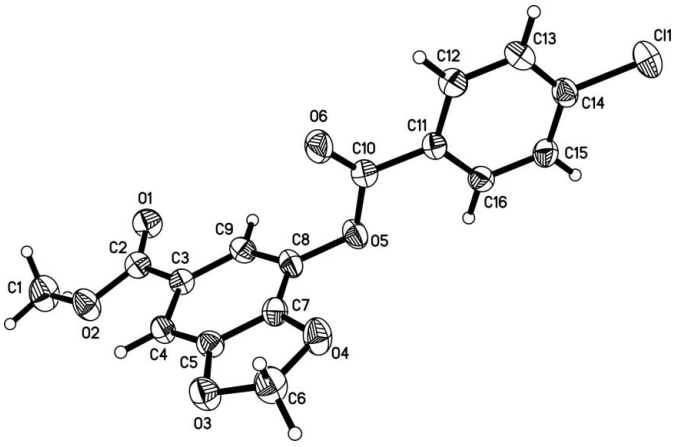


Figure 1
A view of the molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for H atoms).

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.935, T_{max} = 0.961
5956 measured reflections
2625 independent reflections
1494 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
S = 1.00
2625 reflections
209 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 0.1924P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

All H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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