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3,3-Dibenzylbenzo[*b*]furan-2(3*H*)-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.158
Data-to-parameter ratio = 13.9

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

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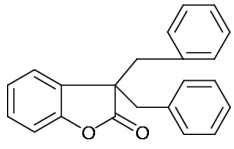
The title compound, $C_{22}H_{18}O_2$, was synthesized by the reaction of methyl (2-hydroxyphenyl)acetate and benzyl chloride. In the crystal structure, the dihydrobenzofuran-2-one ring system lies on a crystallographic mirror plane.

Comment

2,3–Dihydrobenzofuran-2-one derivatives are of great interest because of their biological properties. Some derivatives of 2,3-dihydrobenzofuran-2-one have been reported as potential inhibitors of angiogensis (Duflos *et al.*, 2003) and as drugs for the treatment of hypoxia (Lepagnol & Lavielle, 1988) and some also show high efficacy as intrinsic analgesics and anti-inflammatories (Baumann *et al.*, 1986, Rao & Rau, 1985, Closse *et al.*, 1981). We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1; selected bond lengths and angles are given in Table 1. Atoms C8–C15, O2 and attached H atoms lie on a crystallographic mirror plane..

Experimental

Methyl (2-hydroxyphenyl)acetate (20 mmol) was dissolved in acetone (20 ml) and potassium carbonate (30 mmol) was added in one portion. Benzyl chloride (40 mmol) was then added to this mixture at 293 K. The resulting mixture was refluxed for 20 h. The mixture was filtered and the filtrate concentrated under reduced pressure to afford crude compound (I). Pure (I) was obtained by recrystallization from ethyl acetate (m.p. 454–455 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution. Spectroscopic analysis, ^{1}H NMR ($CDCl_3$, p.p.m.): 7.20–7.21 (*m*, 1H), 7.12–7.15 (*s*, 8H), 6.93–6.95 (*m*, 4H), 6.70–6.72 (*m*, 1H), 3.38–3.41 (*m*, 2H), 3.26–3.28 (*m*, 2H).

Crystal data

$C_{22}H_{18}O_2$
M_r = 314.36
Orthorhombic, *Pnma*
a = 12.650 (3) Å
b = 15.488 (3) Å
c = 8.772 (2) Å
V = 1718.6 (6) Å^3
Z = 4
D_x = 1.215 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25 reflections
θ = 10–13°
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, colourless
0.4 × 0.3 × 0.3 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.973, T_{max} = 0.977
1740 measured reflections
1740 independent reflections
1002 reflections with $I > 2\sigma(I)$
θ_{max} = 26.0°
$h = 0 \rightarrow 15$
$k = 0 \rightarrow 19$
$l = 0 \rightarrow 10$
25 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.158
S = 0.98
1740 reflections
125 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.069 (7)

Table 1
Selected geometric parameters (Å, °).

O1—C9	1.194 (3)	C7—C8	1.550 (2)
O2—C9	1.374 (3)	C8—C15	1.503 (3)
O2—C10	1.404 (3)	C8—C9	1.529 (4)
C4—C7	1.503 (3)	C8—C7^{i}	1.550 (2)
C9—O2—C10	107.8 (2)	C7—C8—C7^{i}	109.4 (2)
C5—C4—C7	121.0 (2)	O1—C9—C8	129.4 (2)
C4—C7—C8	115.1 (2)	O2—C9—C8	110.5 (2)
C15—C8—C9	100.7 (2)	C15—C10—O2	111.9 (2)
C15—C8—C7	113.9 (1)	C10—C15—C8	109.1 (2)
C9—C8—C7	109.3 (1)		

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

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

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL*97.

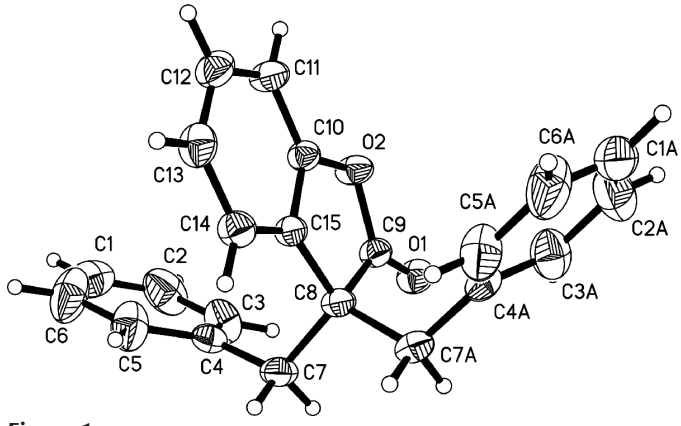


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (A) $x, \frac{1}{2} - y, z$.]

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