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1-[4,5-Bis(benzyloxy)-2-methylphenyl]ethanone

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.009 Å
R factor = 0.061
wR factor = 0.243
Data-to-parameter ratio = 14.0

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

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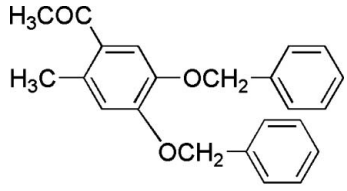
Crystals of the title compound, $C_{23}H_{22}O_3$, were conveniently synthesized according to the method of Patil, Matier & Khuong [(1990). Eur. Patent No. 373592]. The molecule consists of two planar segments that pack to give columns two molecules wide.

Comment

The title compound, (I), is useful in the synthesis of dihydroxybenzoate esters used as antiglaucoma and β-blocking agents. They are useful for the treatment of glaucoma, or for lowering intraocular pressure, since they remain stable when applied topically to the eye but rapidly metabolize as they are absorbed (Patil *et al.*, 1990).



(I)

Compound (I) consists of two major components. The C10–C15 phenyl ring is approximately perpendicular to the mean plane [0.008 (3) Å] through the remaining non-H atoms [dihedral angle between the planes is 87.45 (18)°]. The molecules pack into columns, two molecules wide, with the C8–C20 planar system forming the walls of the column and the C10–C15 phenyl rings extending into the middle of the columns (Fig. 2). Selected bond lengths and angles are listed in Table 1.

Experimental

Compound (I) was obtained by the method of Patil *et al.* (1990). Crystals suitable for structure analysis were obtained by slow evaporation of a solution in a mixture of petroleum ether and acetic acid (8:2) as brown crystalline cubes (m.p. 329–331 K). Elemental analysis calculated: C 79.74, H 6.40%; found: C 79.77, H 6.57%.

Crystal data

$C_{23}H_{22}O_3$
M_r = 346.41
Monoclinic, $P2_1/n$
a = 9.1070 (17) Å
b = 14.681 (3) Å
c = 14.121 (3) Å
β = 99.320 (16)°
V = 1863.1 (7) Å^3
Z = 4
D_x = 1.235 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
Cubic, brown
0.30 × 0.30 × 0.30 mm

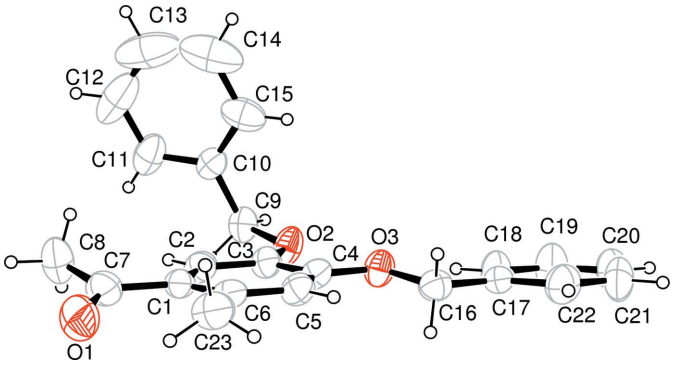


Figure 1
The structure of (I), shown with 30% probability displacement ellipsoids.

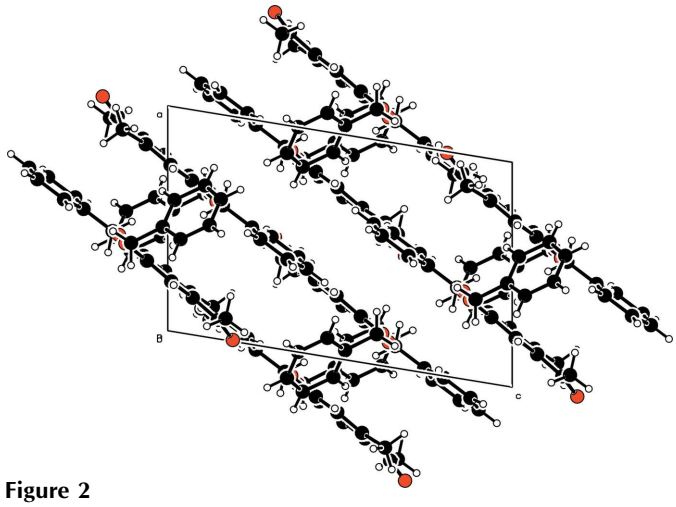


Figure 2
Packing diagram of (I), viewed along the *b* axis, showing the molecules aggregated into columns.

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.945, T_{max} = 0.983
3771 measured reflections
3338 independent reflections
1184 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 25.2°
3 standard reflections
frequency: 60 min
intensity decay: 0.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.243
S = 1.02
3338 reflections
238 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1108P)^2 + 0.1962P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0107 (18)

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.253 (6)	O3—C16	1.435 (5)
O2—C3	1.378 (5)	C7—C8	1.457 (7)
O2—C9	1.420 (5)	C9—C10	1.483 (6)
O3—C4	1.351 (5)	C16—C17	1.489 (6)
C6—C1—C2	120.1 (4)	C8—C7—C1	120.7 (5)
C6—C1—C7	123.4 (5)	O2—C9—C10	113.9 (4)
O1—C7—C8	119.7 (5)	O3—C16—C17	108.9 (4)
O1—C7—C1	119.6 (5)		

H atoms bonded to C atoms were placed in calculated positions and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(parent atom) [or 1.5U_{eq}(methyl C)], with C—H distances of 0.96–0.97 Å, and 0.93 Å for those bonded to benzene rings.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4*, *PSI* and *EAC* (Enraf–Nonius, 1994); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Version 1.05; Farrugia, 1999); software used to prepare material for publication: *SHELXL97*.

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