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Diethyl 4,4′-(butane-1,4-diyldioxy)dibenzoate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.046
wR factor = 0.111
Data-to-parameter ratio = 19.3

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

The title compound, $C_{22}H_{26}O_6$, was synthesized by the reaction of ethyl 4-hydroxybenzoate and 1,4-dichlorobutane. In the slightly bow-shaped molecule with an extended conformation, the dihedral angle between the two benzene rings is 76.02 (7)°.

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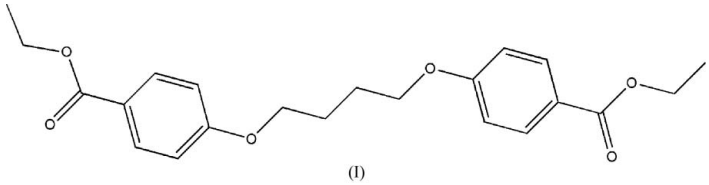
Comment

Ester ligands can stabilize the resulting compounds by coordinating to main group and transition metals (Ríos-Moreno *et al.*, 2003). Much attention has been devoted to the synthesis of new ester ligands. In this work, a diester compound was synthesized and the molecular structure of the title compound, (I), is presented (Fig. 1).



(I)

The molecule has an extended, slightly bow-shaped conformation, the dihedral angle between the two benzene ring being 76.02 (7)°. The bond distances involving O atoms (Table 1) are in agreement with those found in related compounds (Chen *et al.*, 2006; Herrera *et al.*, 2003).

Experimental

A mixture of ethyl 4-hydroxybenzoate (0.83 g, 5 mmol) and NaOH (0.20 g, 5 mmol) in DMF (10 ml) was stirred at 333 K for 1 h, and then 1,4-dichlorobutane (0.32 g, 2.5 mmol) was added. After stirring at 333 K for 2 h, the mixture was cooled to room temperature and then poured into 200 ml of water. A white solid was formed immediately, which was recrystallized from an ethanol–water solution (2:1). Elemental analysis calculated for $C_{22}H_{26}O_6$: C 68.38, H 6.78; found C 68.34, H 6.75%.

Crystal data

$C_{22}H_{26}O_6$
M_r = 386.43
Monoclinic, $P2_1/c$
a = 12.8522 (7) Å
b = 8.3689 (5) Å
c = 19.6835 (11) Å
β = 106.676 (1)°
V = 2028.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.43 × 0.22 × 0.11 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: none
12266 measured reflections
4871 independent reflections
2391 reflections with $I > 2\sigma(I)$
R_{int} = 0.082

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$	253 parameters
$wR(F^2) = 0.111$	H-atom parameters constrained
$S = 0.84$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
4871 reflections	$\Delta\rho_{min} = -0.25$ e Å^{-3}

Table 1
Selected bond lengths (Å).

C2—O1	1.4551 (17)	C13—O4	1.4284 (17)
C3—O2	1.2047 (17)	C15—O4	1.3687 (16)
C3—O1	1.3290 (18)	C20—O5	1.2038 (18)
C7—O3	1.3611 (15)	C20—O6	1.3345 (19)
C10—O3	1.4360 (16)	C21—O6	1.4533 (16)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL-Plus*.

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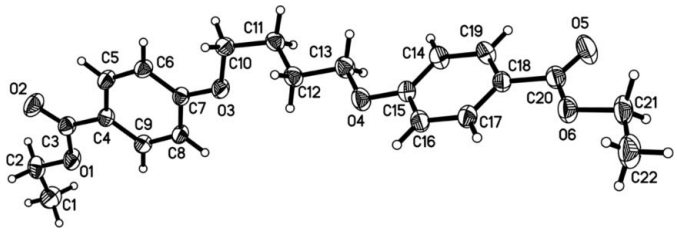

Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

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