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1,4-Bis(3-hydroxymethylphenoxy)butane

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.052
wR factor = 0.156
Data-to-parameter ratio = 15.6

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

The molecule of the title compound, $C_{18}H_{22}O_4$, has a center of symmetry. Molecules are linked into a zigzag chain *via* an O—H···O hydrogen bond. The chains are further linked by O—H···O and C—H···π interactions to form a layer.

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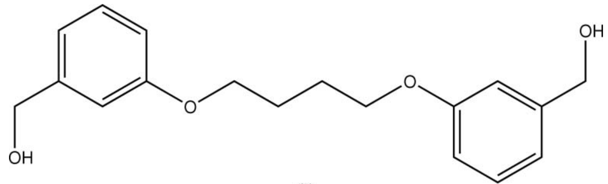
Comment

We have recently reported the structure of 1,6-bis(3-hydroxymethylphenoxy)hexane, (II) (Li *et al.*, 2006). In our ongoing studies of diethers, the title compound, (I), was synthesized and its crystal structure was determined.



(I)

The title molecule has a center of symmetryat the mid-point of the central C—C bond. All bond lengths and angles in (I) (Table 1) show normal ranges (Allen *et al.*, 1987), and are comparable to those in (II). In the crystal structure, molecules are linked into a zigzag chain along the [201] direction by a weak O—H···O hydrogen bond (Fig. 2 and Table 2). The chains are further linked by O—H···O and C–H···π interactions (Table 2), forming a layer parallel to the (201) plane.

Experimental

To a solution of 3-hydroxymethylphenol (1.5 g, 12 mmol) in EtOH (90 ml) was added 10 mol l^{-1} NaOH (1.2 ml, 12 mmol), followed by 1,4-dibromobutane (1.3 g, 6 mmol). The reaction was refluxed for 23 h, cooled to room temperature and diluted with water (30 ml). The brown mixture was subsequently extracted with CH_2Cl_2, and the combined extracts were dried ($MgSO_4$) and concentrated *in vacuo* to give an off-white solid. Purification by flash chromatography (CH_2Cl_2/Me_2CO 4:1, *v*/*v*) gave the title compound as a slightly pink solid. Yellow single crystals were obtained by slow evaporation of an ethyl acetate–ethanol (3:1 *v*/*v*) solution at room temperature over a period of two weeks.

Crystal data

$C_{18}H_{22}O_4$
$M_r = 302.36$
Monoclinic, $P2_1/c$
$a = 13.920$ (3) Å
$b = 4.8454$ (9) Å
$c = 12.846$ (2) Å
$\beta = 112.347$ (3)°
$V = 801.4$ (3) Å^3
$Z = 2$
$D_x = 1.253$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1160 reflections
$\theta = 3.2$–23.7°
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Plate, yellow
0.36 × 0.16 × 0.06 mm

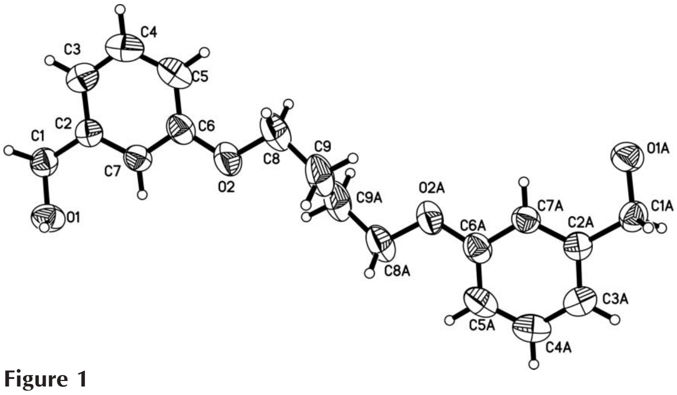


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom numbering scheme. The suffix A corresponds to symmetry code $(1 - x, 2 - y, 2 - z)$.

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min} = 0.969$, $T_{\rm max} = 0.995$
4195 measured reflections
1557 independent reflections
1186 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\rm max} = 26.0°$
$h = -17 \rightarrow 15$
$k = -5 \rightarrow 5$
$l = -15 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.156$
$S = 1.06$
1557 reflections
100 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0758P)^2 + 0.191P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.33$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.27$ e Å^{-3}

Table 1
Selected bond lengths (Å).

O1—C1	1.405 (2)	O2—C8	1.437 (2)
O2—C6	1.367 (3)	C8—C9	1.497 (3)

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C2–C7 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O1$^{\rm i}$	0.82	1.95	2.765 (2)	173
C1—H1*C*···*Cg*1$^{\rm ii}$	0.97	2.76	3.685	160

Symmetry codes: (i) $-x, y + \frac{1}{2}, -z + \frac{3}{2}$; (ii) $x, y - 1, z$.

All H atoms were located in a difference Fourier map and constrained to ride on their parent atoms, with O—H = 0.82 Å and C—H = 0.93–0.97 Å, and with $U_{\rm iso}$(H) = $1.5U_{\rm eq}$(O) and $1.2U_{\rm eq}$(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

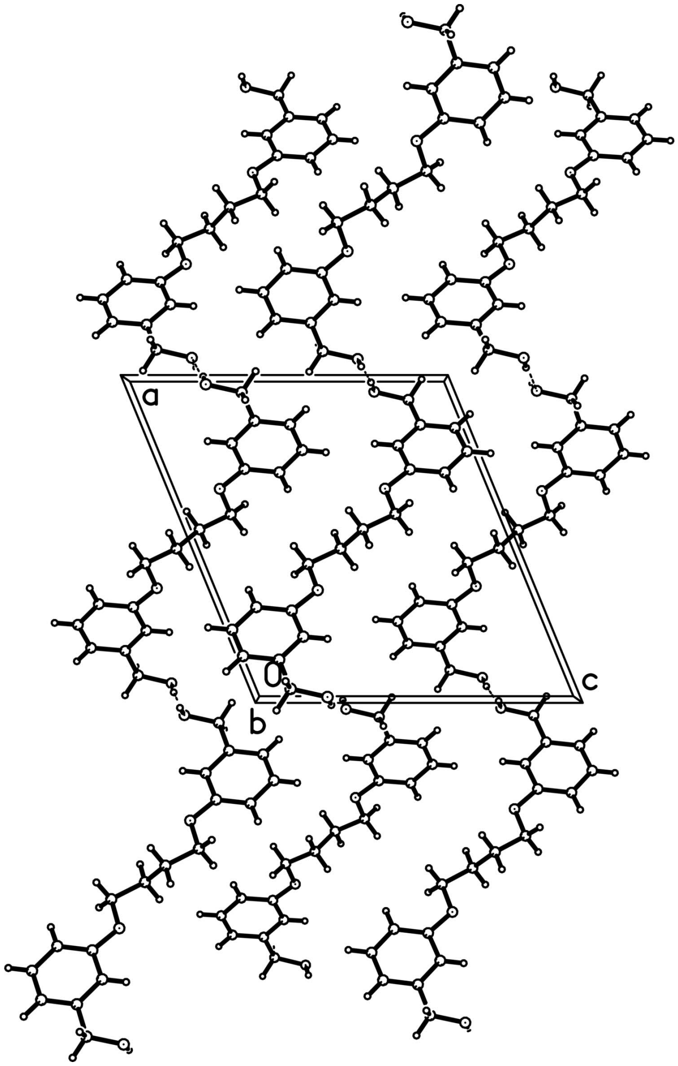


Figure 2
A packing view down the *b* axis. Hydrogen bonds are indicated by dashed lines.

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