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3-[2-(3-Formylphenoxy)ethoxy]benzaldehyde

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.130
Data-to-parameter ratio = 15.0

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, $C_{16}H_{14}O_4$, is nearly planar. A crystallographic centre of symmetry is located at the mid-point of the central C—C bond. The two aromatic rings are parallel to each other. The crystal structure is stabilized by weak intermolecular C—H···O hydrogen bonds.

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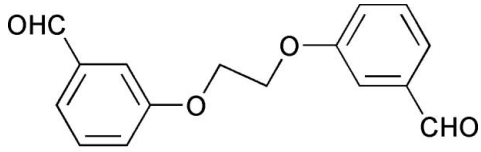
Comment

Since their initial synthesis by Pedersen (1967), crown ethers have been shown to be of great importance in supramolecular chemistry as they can form supramolecular structures which can be used as models for studying weak interactions. Consequently, these species have been used to study the molecular recognition of special guest molecules (Habata *et al.*, 1996). As part of our interest in the molecular and ionic recognition properties of crown ethers, we have now investigated the title compound, (I), used as a precursor in the preparation of crown ethers.



(I)

Fig. 1 shows the molecular structure of (I), with the atomic numbering scheme. In (I), a crystallographic centre of symmetry is located at the mid-point of the central C8—C8^{i} bond [symmetry code: (i) $-x+1, -y+1, -z+2$]. The 3-hydroxybenzaldehyde residue (C1–C7/O2) is essentially planar, with an r.m.s. deviation for the fitted atoms of 0.0159 (19) Å. The two aromatic rings in the molecule are exactly parallel to each other by symmetry. The C8—O2—C1—C6 torsion angle of −172.2 (2)° confirms the nearly

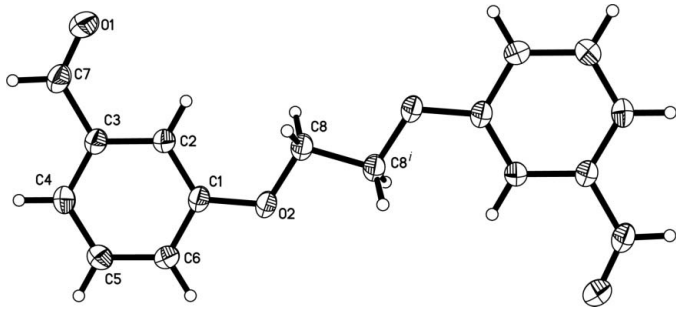


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $-x+1, -y+1, -z+2$.]

planar conformation of the molecule. The geometry is similar to that in 4-[2-(4-formyl-2-methoxyphenoxy)ethoxy]-3-methoxybenzaldehyde (Diao *et al.*, 2005). All bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987).

The crystal structure is stabilized by weak intermolecular C—H···O hydrogen bonds (Table 2 and Fig. 2), forming an infinite framework.

Experimental

1,2-Dibromoethane (9.4 g, 50 mmol) was added dropwise over 0.5 h to a solution of 3-hydroxybenzaldehyde (12.2 g, 100 mmol) and potassium carbonate (13.8 g, 100 mmol) in acetonitrile (500 ml), and the mixture was refluxed for 24 h under nitrogen. The solvent was removed and the resultant mixture poured into ice–water (500 ml). The white precipitate which formed was then isolated and recrystallized from acetonitrile to give the pure compound (yield 6.1 g, 45%; m.p. 364K). Colourless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{16}H_{14}O_4$	D_x = 1.342 Mg m^{-3}
M_r = 270.27	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 1346 reflections
a = 5.6966 (14) Å	θ = 3.1–24.5°
b = 16.098 (4) Å	μ = 0.10 mm^{-1}
c = 7.4113 (18) Å	T = 294 (2) K
β = 100.309 (4)°	Block, colourless
V = 668.7 (3) Å^3	0.36 × 0.22 × 0.14 mm
Z = 2	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	1366 independent reflections
	899 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.032
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 26.4°
	$h = -7 \rightarrow 6$
T_{min} = 0.952, T_{max} = 0.987	$k = -13 \rightarrow 20$
3701 measured reflections	$l = -8 \rightarrow 9$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0734P)^2 + 0.0615P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.043	
$wR(F^2)$ = 0.130	
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
1366 reflections	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
91 parameters	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.205 (2)	O2—C8	1.425 (2)
O2—C1	1.372 (2)		
C1—O2—C8	117.45 (14)	O1—C7—C3	124.65 (18)
O2—C1—C2	124.60 (16)	O2—C8—C8^{i}	105.52 (17)
O2—C1—C6	115.16 (16)		

Symmetry codes: (i) $-x+1, -y+1, -z+2$.

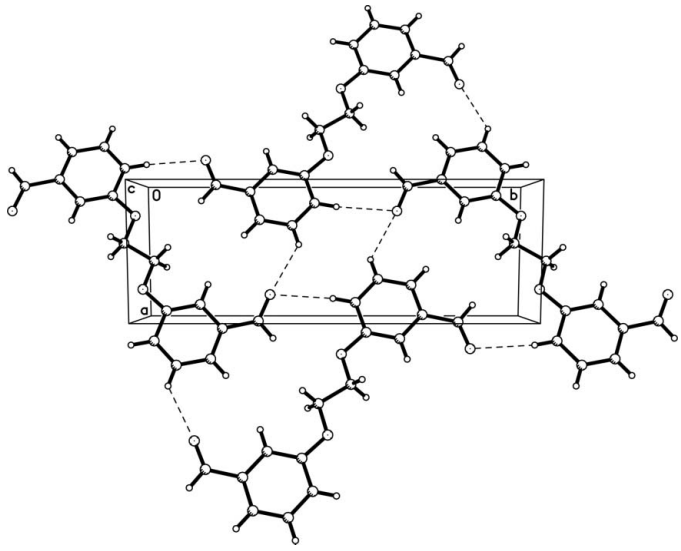


Figure 2
A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O1^{ii}	0.93	2.57	3.475 (2)	163
C5—H5···O1^{iii}	0.93	2.57	3.306 (2)	136

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

H atoms were positioned geometrically and they were constrained to ride on their parent atoms, with C—H distances of 0.93 (CH) and 0.97 Å (CH_2) and with U_{iso}(H) = 1.2U_{eq}(C).

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

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

Bruker (1999). *SMART* (Version 5.0) and *SAINT* (Version 4.0). Bruker AXS Inc., Madison, Wisconsin, USA.

Diao, C.-H., Guo, M.-J., Yu, M., Chen, X., Jing, Z.-L. & Deng, Q.-L. (2005). *Acta Cryst.* E**61**, o3741–o3742.

Habata, Y., Bradshaw, J. S., Young, J. J., Castle, S. L., Huszthy, P., Pyo, T., Lee, M. L. & Izatt, R. (1996). *J. Org. Chem.* **61**, 8391–8396.

Pedersen, C. J. (1967). *J. Am. Chem. Soc.* **89**, 7017–7036.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.