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1,6-Bis(*p*-tolyloxy)hexane

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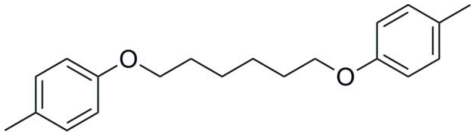
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.077; wR factor = 0.316; data-to-parameter ratio = 15.3.

The title compound, $C_{20}H_{26}O_2$, crystallized with one half-molecule in the asymmetric unit. The whole molecule is generated by inversion symmetry, with the center of inversion being situated at the mid-point of the central $-CH_2-CH_2-$ bond of the bridging hexane chain. In the crystal, molecules stack in columns along the b axis. C—H$\cdots\pi$ interactions are present within the columns.

Related literature

For the properties and synthesis of the title compound, see: Saito *et al.* (1988). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{20}H_{26}O_2$
M_r = 298.41
Monoclinic, $P2_1/c$
a = 18.932 (12) Å
b = 7.327 (4) Å
c = 6.352 (4) Å
β = 91.000 (13)°
V = 881.0 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 K
0.25 × 0.20 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.983, T_{max} = 0.987
4572 measured reflections
1544 independent reflections
963 reflections with $I > 2\sigma(I)$
R_{int} = 0.117
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.316
S = 1.10
1544 reflections
101 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C4—H4$\cdots Cg^{i}$	0.93	2.95	3.696 (4)	138
C7—H7$\cdots Cg^{ii}$	0.93	2.84	3.572 (4)	137

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo,1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SU2725).

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supporting information

Acta Cryst. (2014). E**70**, o617 [doi:10.1107/S1600536814009222]

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S1. Comment

The title compound is used as a sensitizer for thermal recording materials, polyester-resin monomers and fire-resistant materials (Saito *et al.*, 1988).

The molecular structure of the title compound is shown in Fig. 1. The bond lengths (Allen *et al.* (1987) and angles are within normal ranges. It crystallized with half a molecule in the asymmetric unit. The whole molecule is generated by inversion symmetry with the center of inversion being situated at the center of the C10—C10^{i} bond of the bridging hexane chain [symmetry code: (i) -*x*, -*y*, -*z* + 2].

In the crystal, there are no intermolecular hydrogen bonds present (Fig. 2). The molecules stack in columns along the *b* axis and within the columns there are C—H···π interactions present (Table 1).

S2. Experimental

The title compound was prepared by the reported procedure (Saito *et al.*, 1988). Anhydrous potassium carbonate (6.2 g, 45 mmol) was added to a solution of 1,6-dibromohexane (2.5 g, 10.25 mmol) and 4-methoxyphenol (3.18 g, 25.6 mmol) in acetonitrile (100 ml). The mixture was stirred overnight at 338 K, and then filtered and the filtrate evaporated under reduced pressure. The residue was subjected to flash chromatography on silica gel, eluting with (10:1/petroleum ether:ethyl acetate) to give the title compound (Yield 2.13 g). Colourless block-like crystals of the title compound were obtained by slow evaporation of a solution in ethanol (20 ml), after ca. 7 days.

S3. Refinement

All the H atoms were positioned geometrically and constrained to ride on their parent atoms: C—H = 0.93 - 0.97 Å with U_{iso}(H) = 1.5U_{eq}(*C*-methyl) and = 1.2U_{eq}(C) for other H atoms.

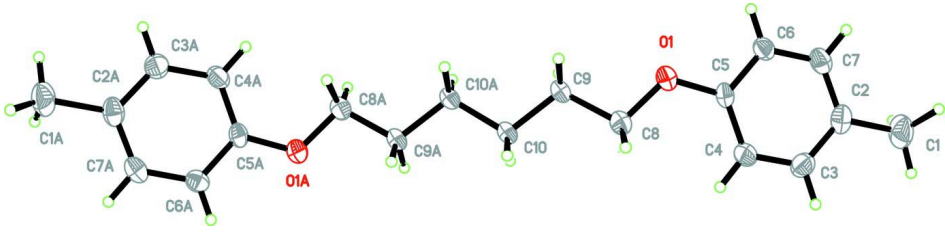

Figure 1

The molecular structure of the title molecule, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

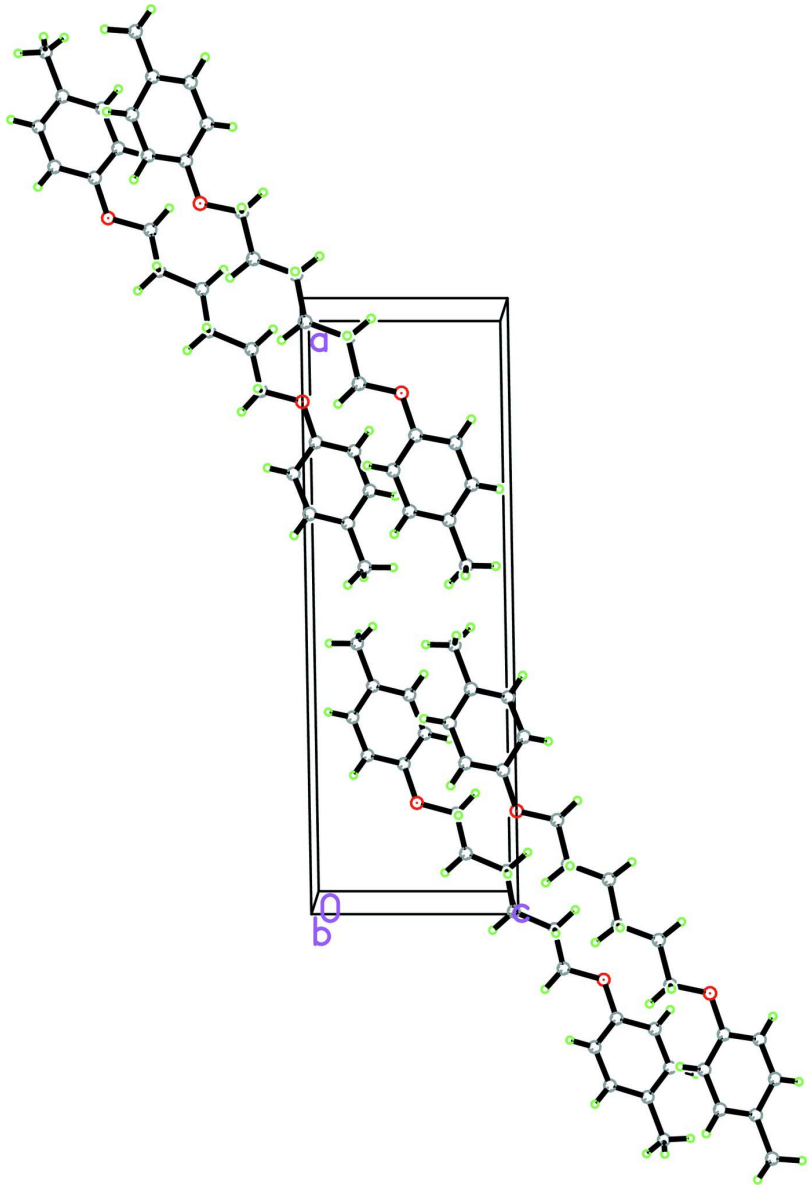

Figure 2

A view along the *b* axis of the crystal packing of the title compound.

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Crystal data

$C_{20}H_{26}O_2$
$M_r = 298.41$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 18.932$ (12) Å
$b = 7.327$ (4) Å
$c = 6.352$ (4) Å
$\beta = 91.000$ (13)°
$V = 881.0$ (9) Å^3
$Z = 2$

$F(000) = 324$
$D_x = 1.125$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1071 reflections
$\theta = 2.2$–23.2°
$\mu = 0.07$ mm^{-1}
$T = 293$ K
Block, colourless
0.25 × 0.20 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.983, T_{max} = 0.987
4572 measured reflections
1544 independent reflections
963 reflections with $I > 2\sigma(I)$
R_{int} = 0.117
θ_{max} = 25.0°, θ_{min} = 1.1°
$h = -22\rightarrow21$
$k = -5\rightarrow8$
$l = -7\rightarrow7$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.316
S = 1.10
1544 reflections
101 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.15451 (11)	−0.0150 (4)	0.5211 (3)	0.0524 (8)
C1	0.4342 (2)	−0.0202 (7)	0.2221 (7)	0.0812 (15)
H1A	0.4508	−0.1439	0.2302	0.122*
H1B	0.4644	0.0567	0.3067	0.122*
H1C	0.4349	0.0203	0.0784	0.122*
C2	0.36013 (17)	−0.0103 (5)	0.3018 (6)	0.0535 (10)
C3	0.34523 (17)	0.0740 (5)	0.4910 (6)	0.0555 (10)
H3	0.3819	0.1277	0.5682	0.067*
C4	0.27798 (16)	0.0806 (5)	0.5681 (5)	0.0497 (10)
H4	0.2691	0.1409	0.6937	0.060*
C5	0.22302 (16)	−0.0041 (4)	0.4560 (5)	0.0400 (9)
C6	0.23675 (16)	−0.0871 (5)	0.2660 (4)	0.0439 (9)
H6	0.2002	−0.1416	0.1892	0.053*
C7	0.30380 (17)	−0.0892 (5)	0.1906 (5)	0.0502 (10)
H7	0.3121	−0.1448	0.0618	0.060*

C8	0.13751 (15)	0.0427 (5)	0.7259 (5)	0.0456 (9)
H8A	0.1378	0.1749	0.7336	0.055*
H8B	0.1719	−0.0042	0.8273	0.055*
C9	0.06519 (15)	−0.0294 (5)	0.7732 (4)	0.0449 (9)
H9A	0.0669	−0.1617	0.7745	0.054*
H9B	0.0327	0.0074	0.6612	0.054*
C10	0.03691 (14)	0.0366 (5)	0.9817 (4)	0.0403 (9)
H10A	0.0358	0.1690	0.9826	0.048*
H10B	0.0682	−0.0032	1.0951	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0479 (16)	0.0683 (18)	0.0413 (14)	−0.0032 (10)	0.0101 (10)	−0.0063 (11)
C1	0.064 (3)	0.093 (4)	0.088 (3)	0.002 (2)	0.034 (2)	−0.005 (3)
C2	0.053 (2)	0.043 (2)	0.065 (2)	0.0025 (15)	0.0202 (17)	0.0055 (17)
C3	0.051 (2)	0.051 (2)	0.065 (2)	−0.0086 (16)	0.0069 (16)	−0.0079 (18)
C4	0.055 (2)	0.049 (2)	0.0456 (18)	−0.0020 (15)	0.0089 (15)	−0.0109 (16)
C5	0.0429 (18)	0.0390 (19)	0.0385 (18)	0.0012 (13)	0.0136 (13)	0.0055 (13)
C6	0.0538 (19)	0.043 (2)	0.0346 (16)	−0.0022 (14)	0.0030 (13)	0.0022 (14)
C7	0.065 (2)	0.043 (2)	0.0433 (18)	0.0040 (16)	0.0137 (15)	−0.0009 (15)
C8	0.0469 (19)	0.049 (2)	0.0411 (18)	0.0042 (14)	0.0062 (14)	−0.0022 (14)
C9	0.0475 (19)	0.053 (2)	0.0341 (17)	−0.0005 (14)	0.0093 (13)	−0.0078 (14)
C10	0.0457 (19)	0.046 (2)	0.0297 (16)	0.0024 (13)	0.0059 (13)	−0.0025 (12)

Geometric parameters (Å, º)

O1—C5	1.371 (3)	C6—C7	1.365 (4)
O1—C8	1.410 (4)	C6—H6	0.9300
C1—C2	1.502 (4)	C7—H7	0.9300
C1—H1A	0.9600	C8—C9	1.503 (4)
C1—H1B	0.9600	C8—H8A	0.9700
C1—H1C	0.9600	C8—H8B	0.9700
C2—C3	1.385 (5)	C9—C10	1.516 (4)
C2—C7	1.394 (5)	C9—H9A	0.9700
C3—C4	1.373 (4)	C9—H9B	0.9700
C3—H3	0.9300	C10—C10^{i}	1.519 (5)
C4—C5	1.396 (5)	C10—H10A	0.9700
C4—H4	0.9300	C10—H10B	0.9700
C5—C6	1.380 (4)		
C5—O1—C8	119.6 (2)	C6—C7—C2	121.7 (3)
C2—C1—H1A	109.5	C6—C7—H7	119.2
C2—C1—H1B	109.5	C2—C7—H7	119.2
H1A—C1—H1B	109.5	O1—C8—C9	107.6 (3)
C2—C1—H1C	109.5	O1—C8—H8A	110.2
H1A—C1—H1C	109.5	C9—C8—H8A	110.2
H1B—C1—H1C	109.5	O1—C8—H8B	110.2

C3—C2—C7	117.3 (3)	C9—C8—H8B	110.2
C3—C2—C1	121.3 (4)	H8A—C8—H8B	108.5
C7—C2—C1	121.3 (3)	C8—C9—C10	113.5 (3)
C4—C3—C2	122.0 (3)	C8—C9—H9A	108.9
C4—C3—H3	119.0	C10—C9—H9A	108.9
C2—C3—H3	119.0	C8—C9—H9B	108.9
C3—C4—C5	119.3 (3)	C10—C9—H9B	108.9
C3—C4—H4	120.3	H9A—C9—H9B	107.7
C5—C4—H4	120.3	C9—C10—C10^{i}	111.2 (3)
O1—C5—C6	115.6 (3)	C9—C10—H10A	109.4
O1—C5—C4	124.9 (3)	C10^{i}—C10—H10A	109.4
C6—C5—C4	119.5 (3)	C9—C10—H10B	109.4
C7—C6—C5	120.2 (3)	C10^{i}—C10—H10B	109.4
C7—C6—H6	119.9	H10A—C10—H10B	108.0
C5—C6—H6	119.9		

C7—C2—C3—C4	0.0 (5)	C4—C5—C6—C7	1.3 (5)
C1—C2—C3—C4	−178.6 (4)	C5—C6—C7—C2	0.6 (5)
C2—C3—C4—C5	1.8 (5)	C3—C2—C7—C6	−1.2 (5)
C8—O1—C5—C6	171.1 (3)	C1—C2—C7—C6	177.4 (4)
C8—O1—C5—C4	−7.9 (5)	C5—O1—C8—C9	−165.3 (3)
C3—C4—C5—O1	176.6 (3)	O1—C8—C9—C10	−174.7 (3)
C3—C4—C5—C6	−2.4 (5)	C8—C9—C10—C10^{i}	178.6 (3)
O1—C5—C6—C7	−177.8 (3)		

Symmetry code: (i) −*x*, −*y*, −*z*+2.

Hydrogen-bond geometry (Å, º)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···*Cg*^{ii}	0.93	2.95	3.696 (4)	138
C7—H7···*Cg*^{iii}	0.93	2.84	3.572 (4)	137

Symmetry codes: (ii) *x*, −*y*+1/2, *z*+1/2; (iii) *x*, −*y*−1/2, *z*−1/2.