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1,2-Bis(4-methylphenoxy)ethane

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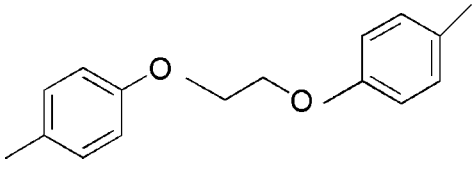
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.057; wR factor = 0.131; data-to-parameter ratio = 15.6.

In the title compound, $C_{16}H_{18}O_2$, the two aromatic rings are almost orthogonal, making a dihedral angle of 89.41 (2)°. There is a C—H$\cdots\pi$ contact between the methylene group and the 4-methylphenyl ring. The molecule exhibits twofold symmetry..

Related literature

For background to the uses of the title compound and further synthetic details, see: Xiao *et al.* (2007).



Experimental

Crystal data

$C_{16}H_{18}O_2$
M_r = 242.30
Monoclinic, $C2/c$
a = 27.173 (5) Å
b = 5.5510 (11) Å
c = 9.2780 (19) Å
β = 93.55 (3)°
V = 1396.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.30 × 0.30 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.978, T_{max} = 0.996
2542 measured reflections
1276 independent reflections
636 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.131
S = 1.00
1276 reflections
82 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

*Cg*1 is the centroid of the 4-methylphenyl ring (C1–C6).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C8—H8$A\cdots Cg$1	0.97	2.85	3.664 (3)	142

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; 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: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5032).

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Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Xiao, X., Sun, J., Li, X., Li, H. & Wang, Y. (2007). *J. Mol. Catal. A*, **267**, 86–91.

supporting information

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1,2-Bis(4-methylphenoxy)ethane

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S1. Experimental

p-Cresol (30.3 g,0.28 mol) was added to a stirred solution of sodium hydroxide(16 g,0.4 mol) in 200 ml of ethanol at room temperature. After stirring for 1 h, ethylene dibromide(28.1 g,0.15 mol) was added. The reaction mixture was stirred and heated under refluxing for another 15 h and then poured into a 5% aqueous solution of NaOH (500 ml). The resulting mixture was cooled to room temperature and filtered. The remaining solid was washed with water(2 *x* 50 ml) and ethanol(2 *x* 40 ml),and then dried *in vacuo* to give the products 13.6 g as white solids (40.1%) (Xiao *et al.*, 2007) Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

S2. Refinement

H atoms were positioned geometrically with C—H = 0.93, 0.98 and 0.97 Å for aromatic, methine and methylene H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 (or 1.5 for methyl groups) times U_{eq}(C).

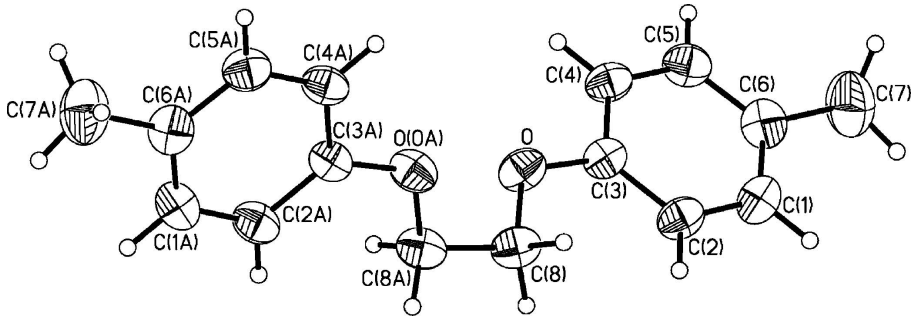

Figure 1

The molecular structure of the title molecule, with the atom numbering scheme. Displacement ellipsoids are drawn at 30% probability levels.

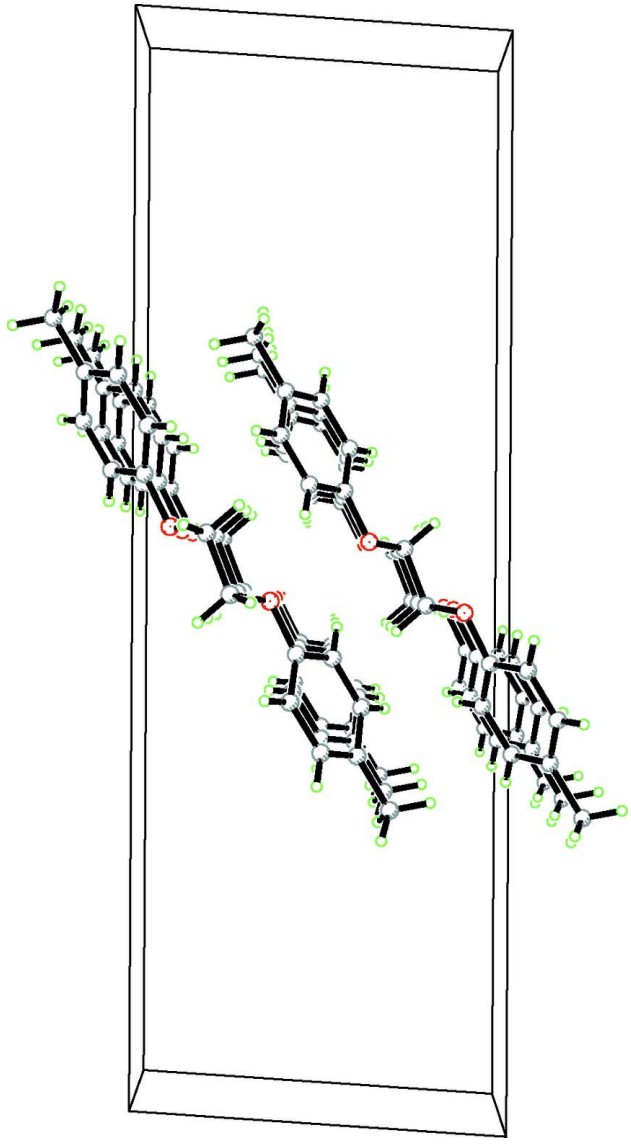

Figure 2

A practical packing diagram of the title compound. There is no intramolecular or intermolecular hydrogen bonds in the crystal.

1-methyl-4-[2-(4-methylphenoxy)ethoxy]benzene

Crystal data

$C_{16}H_{18}O_2$
$M_r = 242.30$
Monoclinic, $C2/c$
$a = 27.173\ (5)$ Å
$b = 5.5510\ (11)$ Å
$c = 9.2780\ (19)$ Å
$\beta = 93.55\ (3)°$
$V = 1396.8\ (5)$ Å^3
$Z = 4$

$F(000) = 520$
$D_x = 1.152$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9–12°$
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Prism, colorless
0.30 × 0.30 × 0.05 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} = 0.978, T_{max} = 0.996
2542 measured reflections
1276 independent reflections
636 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 25.3°, θ_{min} = 1.5°
$h = -32 \rightarrow 32$
$k = 0 \rightarrow 6$
$l = -11 \rightarrow 11$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.131
S = 1.00
1276 reflections
82 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
$w = 1/[\sigma^2(F_o^2) + (0.022P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 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}
O	0.52863 (6)	0.2044 (3)	0.12559 (15)	0.0667 (6)
C1	0.65274 (9)	0.1203 (6)	−0.0026 (3)	0.0768 (9)
H1A	0.6793	0.0147	0.0075	0.092*
C2	0.61155 (9)	0.0757 (5)	0.0739 (2)	0.0660 (7)
H2A	0.6105	−0.0578	0.1342	0.079*
C3	0.57211 (9)	0.2313 (5)	0.0597 (2)	0.0543 (6)
C4	0.57452 (9)	0.4268 (5)	−0.0305 (2)	0.0635 (7)
H4A	0.5479	0.5321	−0.0411	0.076*
C5	0.61569 (10)	0.4681 (5)	−0.1049 (3)	0.0704 (8)
H5A	0.6166	0.6022	−0.1647	0.085*
C6	0.65576 (10)	0.3158 (6)	−0.0932 (3)	0.0752 (9)
C7	0.70126 (10)	0.3646 (6)	−0.1759 (3)	0.1183 (13)
H7A	0.7254	0.2418	−0.1539	0.177*
H7B	0.7147	0.5190	−0.1485	0.177*
H7C	0.6924	0.3637	−0.2777	0.177*

C8	0.52487 (8)	0.0048 (5)	0.2210 (2)	0.0663 (8)
H8A	0.5499	0.0169	0.2998	0.080*
H8B	0.5300	−0.1444	0.1696	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O	0.0811 (12)	0.0665 (12)	0.0532 (9)	0.0140 (11)	0.0085 (9)	0.0125 (11)
C1	0.0708 (18)	0.082 (2)	0.0774 (18)	0.0161 (17)	0.0044 (15)	−0.001 (2)
C2	0.0797 (17)	0.0638 (18)	0.0538 (14)	0.0115 (17)	−0.0030 (13)	0.0044 (16)
C3	0.0670 (16)	0.0574 (16)	0.0382 (12)	0.0066 (15)	−0.0003 (12)	−0.0046 (13)
C4	0.0806 (18)	0.0546 (17)	0.0548 (13)	0.0090 (15)	0.0012 (13)	0.0019 (16)
C5	0.0858 (19)	0.0658 (19)	0.0595 (15)	−0.0035 (17)	0.0023 (15)	0.0060 (17)
C6	0.0771 (19)	0.087 (2)	0.0617 (16)	−0.0028 (19)	0.0093 (15)	−0.006 (2)
C7	0.088 (2)	0.152 (4)	0.118 (2)	−0.005 (2)	0.0279 (19)	0.008 (3)
C8	0.0914 (19)	0.0611 (16)	0.0462 (12)	0.0077 (15)	0.0023 (12)	0.0064 (14)

Geometric parameters (Å, º)

O—C3	1.372 (2)	C5—C6	1.377 (4)
O—C8	1.426 (3)	C5—H5A	0.9300
C1—C6	1.378 (4)	C6—C7	1.519 (3)
C1—C2	1.384 (3)	C7—H7A	0.9600
C1—H1A	0.9300	C7—H7B	0.9600
C2—C3	1.376 (3)	C7—H7C	0.9600
C2—H2A	0.9300	C8—C8^{i}	1.485 (4)
C3—C4	1.375 (3)	C8—H8A	0.9700
C4—C5	1.370 (3)	C8—H8B	0.9700
C4—H4A	0.9300		
C3—O—C8	117.25 (18)	C1—C6—C5	117.0 (3)
C6—C1—C2	122.3 (3)	C1—C6—C7	122.0 (3)
C6—C1—H1A	118.9	C5—C6—C7	121.0 (3)
C2—C1—H1A	118.9	C6—C7—H7A	109.5
C3—C2—C1	119.2 (3)	C6—C7—H7B	109.5
C3—C2—H2A	120.4	H7A—C7—H7B	109.5
C1—C2—H2A	120.4	C6—C7—H7C	109.5
O—C3—C4	115.6 (2)	H7A—C7—H7C	109.5
O—C3—C2	125.2 (2)	H7B—C7—H7C	109.5
C4—C3—C2	119.2 (2)	O—C8—C8^{i}	109.05 (18)
C5—C4—C3	120.7 (3)	O—C8—H8A	109.9
C5—C4—H4A	119.7	C8^{i}—C8—H8A	109.9
C3—C4—H4A	119.7	O—C8—H8B	109.9
C4—C5—C6	121.6 (3)	C8^{i}—C8—H8B	109.9
C4—C5—H5A	119.2	H8A—C8—H8B	108.3
C6—C5—H5A	119.2		
C6—C1—C2—C3	−0.1 (4)	C3—C4—C5—C6	0.5 (4)

C8—O—C3—C4	−179.46 (19)	C2—C1—C6—C5	0.1 (4)
C8—O—C3—C2	2.8 (3)	C2—C1—C6—C7	179.5 (2)
C1—C2—C3—O	177.9 (2)	C4—C5—C6—C1	−0.3 (4)
C1—C2—C3—C4	0.2 (3)	C4—C5—C6—C7	−179.7 (3)
O—C3—C4—C5	−178.3 (2)	C3—O—C8—C8^{i}	−179.03 (19)
C2—C3—C4—C5	−0.4 (3)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···*Cg*1	0.97	2.85	3.664 (3)	142