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# 1,10-Bis[2-(prop-1-enyl)phenoxy]decane

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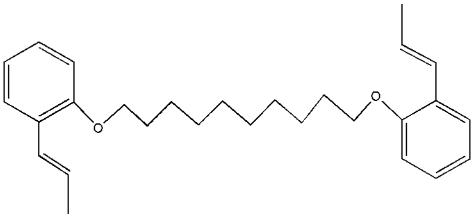
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.069; $wR$ factor = 0.245; data-to-parameter ratio = 22.5.

The complete molecule of the title compound, $C_{28}H_{38}O_2$, is generated by a crystallographic centre of symmetry. The molecular conformation displays an intramolecular C—H⋯$\pi$ interaction.

## Related literature

For general background to the synthesis, see: Wadher *et al.* (2009). For the use of cross-linked polymers in the synthesis of multifunctional monomers, see: Starvin & Rao (2004). For their applications as polymeric sorbents and in the preparation of laser composites, see: Kazuya *et al.* (2000); Ryusuke & Kazufumi (2001). For a related structure, see: Bayramov *et al.* (2011).



## Experimental

### *Crystal data*

$C_{28}H_{38}O_2$
$M_r$ = 406.58
Monoclinic, $P2_1/c$
$a$ = 5.4084 (6) Å
$b$ = 12.2076 (14) Å
$c$ = 19.391 (2) Å
$\beta$ = 92.025 (2)°
$V$ = 1279.5 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.06 mm$^{-1}$
$T$ = 296 K
0.30 × 0.20 × 0.20 mm

### *Data collection*

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
$T_{\min}$ = 0.981, $T_{\max}$ = 0.987
13946 measured reflections
3057 independent reflections
1914 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.025

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.245
$S$ = 1.00
3057 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.60 e Å$^{-3}$
$\Delta\rho_{\min}$ = −0.26 e Å$^{-3}$

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

*Cg*1 is the centroid of the C1–C6 ring.

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| C7—H7$B$⋯$Cg$1 | 0.97 | 2.65 | 2.396 (3) | 143 |

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2373).

## References

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o266 [ **doi:10.1107/S1600536811055061** ]

# 1,10-Bis[2-(prop-1-enyl)phenoxy]decane

**A. M. Maharramov, M. R. Bayramov, G. M. Mehdiyeva, S. B. Hoseinzadeh** and **B. A. Rashidov**

## Comment

Operational cross-linked polymers have been used for synthesis of multifunctional monomers (Starvin *et al.* (2004). These polymers are useful in many applications such as polymeric sorbents and preparing the laser composites (Kazuya *et al.*, 2000); Ryusuke & Kazufumi (2001). In practice, for obtaining polymers of improved functional properties, polymerical transformations are carried out. However, preparation of such cross-linked copolymers have some difficulties related to monomers high reactivity (for example, divinybenzene) and other physico-chemical properties. Therefore, synthesis of multifunctional monomers based on the alkenylphenols is rather important. The authors were synthesised the multifunctional monomers (Bayramov *et al.*, 2011), that can be used in preparation of cross-linked copolymers as a sorbent for heavy metals.

The molecule of title compound, $C_{28}H_{38}O_2$, (I), reveals a crystallographic inversion centre at the mid-point of the central C—C bond (Fig. 1). An asymmetric unit comprises a half of the molecule. The crystal packing displays intramolecular C—H···O hydrogen bonds and C—H···π interaction (Fig. 2, Table 1). The molecule has long chain of ($CH_2$) groups, and so, the polymers based on this monomer are capable to adsorbed heavy metal ions.

## Experimental

2-Propenylphenol (0.015 mol, 2 g) and KOH (0.015 mol, 0.84 g) were dissolved in 6 mL of 2-propanol, then 1,10-dibromedecane (0.006 mol, 1.8 g) was added to this solution. This mixture was stirred at 353 K for 30 m. The desired compounds with yield 2.43 g (99.1%) was filtered and washed with acetone and recrystallised to obtain colourless crystals. $T_{mp}$ = 326 K. The structure of the reported compound - 1,10-bis{2(1-propenyl)phenoxy}decane, was also proved by NMR-spectroscopy. FT-NMR (acetone-$d^6$, p.p.m.), $^1$H: 1.92 d (6*H*,$CH_3$); 2.05 t (4*H*, $CH_2$); 4.16 t (4*H*, $OCH_2$); 6.13 m (2*H*, CH=); 6.67–7.2 m (8*H*, 2Ar); 7.3 d (2*H*,CH=). $^{13}$C: 18.5; 26.1; 67.1; 112.3; 121.4; 124.4; 126.0; 127.1; 127.3; 127.5; 156.0.

## Refinement

The hydrogen atoms were placed at calculated positions and refined in the riding mode with fixed isotropic displacement parameters [$U_{iso}$(H) = 1.2Ueq(C)].

## Figures

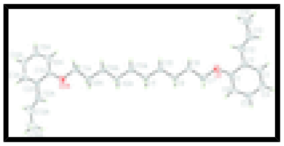

Fig. 1. The molecular structure of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

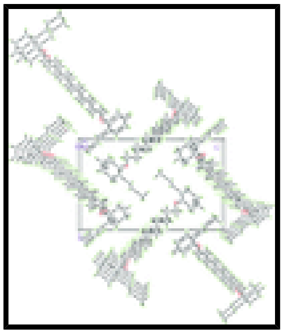

Fig. 2. Packing of chains in the unit cell.

### 1,10-Bis[2-(prop-1-enyl)phenoxy]decane

*Crystal data*

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$M_r = 406.58$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 5.4084$ (6) Å

$b = 12.2076$ (14) Å

$c = 19.391$ (2) Å

$\beta = 92.025$ (2)°

$V = 1279.5$ (3) Å$^3$

$Z = 2$

$F(000) = 444$

$D_x = 1.055$ Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3093 reflections

$\theta = 2.7–25.5°$

$\mu = 0.06$ mm$^{-1}$

$T = 296$ K

Prism, colourless

0.30 × 0.20 × 0.20 mm

*Data collection*

Bruker APEXII CCD diffractometer

Radiation source: fine-focus sealed tube

graphite

phi and $\omega$ scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)

$T_{\min} = 0.981$, $T_{\max} = 0.987$

13946 measured reflections

3057 independent reflections

1914 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 28.0°$, $\theta_{\min} = 2.0°$

$h = -7 \rightarrow 7$

$k = -16 \rightarrow 16$

$l = -25 \rightarrow 25$

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.069$

$wR(F^2) = 0.245$

$S = 1.00$

3057 reflections

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1494P)^2 + 0.1404P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

| | |
|---|---|
| 136 parameters | $\Delta\rho_{\max} = 0.60$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{\min} = -0.26$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{\rm iso}$*/$U_{\rm eq}$ |
|---|---|---|---|---|
| O1 | 0.3626 (3) | 0.30774 (11) | 0.33897 (7) | 0.0679 (4) |
| C1 | 0.5218 (3) | 0.32178 (16) | 0.28696 (10) | 0.0594 (5) |
| C2 | 0.6858 (4) | 0.41008 (15) | 0.29461 (11) | 0.0623 (5) |
| C3 | 0.8580 (4) | 0.42419 (19) | 0.24299 (13) | 0.0759 (6) |
| H3A | 0.9706 | 0.4816 | 0.2470 | 0.091* |
| C4 | 0.8663 (5) | 0.3562 (2) | 0.18664 (13) | 0.0807 (7) |
| H4A | 0.9832 | 0.3675 | 0.1533 | 0.097* |
| C5 | 0.7018 (5) | 0.2721 (2) | 0.18001 (12) | 0.0801 (7) |
| H5A | 0.7052 | 0.2265 | 0.1417 | 0.096* |
| C6 | 0.5292 (4) | 0.25403 (19) | 0.23007 (10) | 0.0709 (6) |
| H6A | 0.4182 | 0.1961 | 0.2253 | 0.085* |
| C7 | 0.2015 (3) | 0.21479 (15) | 0.33632 (10) | 0.0583 (5) |
| H7A | 0.2977 | 0.1480 | 0.3336 | 0.070* |
| H7B | 0.0917 | 0.2190 | 0.2958 | 0.070* |
| C8 | 0.0534 (3) | 0.21399 (15) | 0.40044 (10) | 0.0569 (5) |
| H8A | −0.0470 | 0.2797 | 0.4018 | 0.068* |
| H8B | 0.1649 | 0.2142 | 0.4407 | 0.068* |
| C9 | −0.1122 (3) | 0.11440 (15) | 0.40254 (9) | 0.0573 (5) |
| H9A | −0.0101 | 0.0492 | 0.4008 | 0.069* |
| H9B | −0.2211 | 0.1145 | 0.3617 | 0.069* |
| C10 | −0.2681 (3) | 0.10799 (15) | 0.46559 (10) | 0.0572 (5) |
| H10A | −0.3772 | 0.1710 | 0.4661 | 0.069* |
| H10B | −0.1602 | 0.1116 | 0.5066 | 0.069* |
| C11 | −0.4231 (3) | 0.00446 (16) | 0.46864 (10) | 0.0590 (5) |
| H11A | −0.5320 | 0.0015 | 0.4279 | 0.071* |
| H11B | −0.3137 | −0.0584 | 0.4673 | 0.071* |
| C12 | 0.6767 (5) | 0.48117 (17) | 0.35572 (13) | 0.0801 (7) |
| H12A | 0.5316 | 0.4780 | 0.3800 | 0.096* |
| C13 | 0.8412 (7) | 0.5460 (2) | 0.37940 (17) | 0.1110 (10) |
| H13A | 0.9898 | 0.5505 | 0.3569 | 0.133* |

| | | | | |
|---|---|---|---|---|
| C14 | 0.8081 (10) | 0.6169 (3) | 0.4428 (2) | 0.1568 (18) |
| H14A | 0.9548 | 0.6596 | 0.4516 | 0.235* |
| H14B | 0.7791 | 0.5710 | 0.4819 | 0.235* |
| H14C | 0.6693 | 0.6649 | 0.4350 | 0.235* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0720 (9) | 0.0654 (8) | 0.0673 (9) | −0.0168 (7) | 0.0141 (7) | −0.0044 (6) |
| C1 | 0.0610 (11) | 0.0573 (10) | 0.0602 (10) | −0.0039 (8) | 0.0041 (8) | 0.0110 (8) |
| C2 | 0.0671 (11) | 0.0512 (10) | 0.0685 (11) | −0.0033 (8) | 0.0004 (9) | 0.0138 (8) |
| C3 | 0.0764 (13) | 0.0648 (12) | 0.0871 (15) | −0.0092 (10) | 0.0102 (11) | 0.0256 (11) |
| C4 | 0.0881 (16) | 0.0832 (15) | 0.0720 (14) | 0.0012 (12) | 0.0210 (12) | 0.0203 (11) |
| C5 | 0.0949 (17) | 0.0840 (15) | 0.0622 (12) | −0.0005 (13) | 0.0131 (11) | 0.0034 (10) |
| C6 | 0.0767 (13) | 0.0731 (13) | 0.0631 (12) | −0.0117 (10) | 0.0051 (10) | 0.0010 (9) |
| C7 | 0.0580 (10) | 0.0544 (10) | 0.0625 (10) | −0.0083 (8) | 0.0034 (8) | 0.0039 (8) |
| C8 | 0.0544 (10) | 0.0550 (10) | 0.0613 (10) | −0.0001 (8) | 0.0049 (8) | 0.0041 (8) |
| C9 | 0.0514 (10) | 0.0606 (10) | 0.0599 (10) | −0.0024 (8) | 0.0044 (8) | 0.0050 (8) |
| C10 | 0.0482 (9) | 0.0611 (10) | 0.0626 (10) | −0.0007 (8) | 0.0062 (8) | 0.0055 (8) |
| C11 | 0.0486 (10) | 0.0647 (11) | 0.0640 (11) | −0.0019 (8) | 0.0066 (8) | 0.0067 (8) |
| C12 | 0.0940 (17) | 0.0545 (11) | 0.0915 (16) | −0.0099 (11) | 0.0002 (13) | 0.0077 (10) |
| C13 | 0.122 (2) | 0.0941 (19) | 0.116 (2) | −0.0182 (18) | −0.0054 (19) | −0.0093 (16) |
| C14 | 0.229 (5) | 0.101 (2) | 0.137 (3) | −0.006 (3) | −0.048 (3) | −0.037 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.360 (2) | C8—H8B | 0.9700 |
| O1—C7 | 1.430 (2) | C9—C10 | 1.511 (2) |
| C1—C6 | 1.380 (3) | C9—H9A | 0.9700 |
| C1—C2 | 1.401 (3) | C9—H9B | 0.9700 |
| C2—C3 | 1.402 (3) | C10—C11 | 1.519 (3) |
| C2—C12 | 1.471 (3) | C10—H10A | 0.9700 |
| C3—C4 | 1.374 (4) | C10—H10B | 0.9700 |
| C3—H3A | 0.9300 | C11—C11$^{i}$ | 1.502 (4) |
| C4—C5 | 1.361 (4) | C11—H11A | 0.9700 |
| C4—H4A | 0.9300 | C11—H11B | 0.9700 |
| C5—C6 | 1.388 (3) | C12—C13 | 1.265 (4) |
| C5—H5A | 0.9300 | C12—H12A | 0.9300 |
| C6—H6A | 0.9300 | C13—C14 | 1.519 (5) |
| C7—C8 | 1.503 (3) | C13—H13A | 0.9300 |
| C7—H7A | 0.9700 | C14—H14A | 0.9600 |
| C7—H7B | 0.9700 | C14—H14B | 0.9600 |
| C8—C9 | 1.511 (3) | C14—H14C | 0.9600 |
| C8—H8A | 0.9700 | | |
| C1—O1—C7 | 118.31 (15) | C8—C9—C10 | 114.29 (16) |
| O1—C1—C6 | 123.66 (17) | C8—C9—H9A | 108.7 |
| O1—C1—C2 | 115.70 (17) | C10—C9—H9A | 108.7 |
| C6—C1—C2 | 120.63 (18) | C8—C9—H9B | 108.7 |

| | | | |
|---|---|---|---|
| C1—C2—C3 | 116.96 (19) | C10—C9—H9B | 108.7 |
| C1—C2—C12 | 120.00 (19) | H9A—C9—H9B | 107.6 |
| C3—C2—C12 | 123.02 (19) | C9—C10—C11 | 113.51 (16) |
| C4—C3—C2 | 122.3 (2) | C9—C10—H10A | 108.9 |
| C4—C3—H3A | 118.8 | C11—C10—H10A | 108.9 |
| C2—C3—H3A | 118.8 | C9—C10—H10B | 108.9 |
| C5—C4—C3 | 119.4 (2) | C11—C10—H10B | 108.9 |
| C5—C4—H4A | 120.3 | H10A—C10—H10B | 107.7 |
| C3—C4—H4A | 120.3 | C11$^{\rm i}$—C11—C10 | 114.5 (2) |
| C4—C5—C6 | 120.5 (2) | C11$^{\rm i}$—C11—H11A | 108.6 |
| C4—C5—H5A | 119.8 | C10—C11—H11A | 108.6 |
| C6—C5—H5A | 119.8 | C11$^{\rm i}$—C11—H11B | 108.6 |
| C1—C6—C5 | 120.2 (2) | C10—C11—H11B | 108.6 |
| C1—C6—H6A | 119.9 | H11A—C11—H11B | 107.6 |
| C5—C6—H6A | 119.9 | C13—C12—C2 | 128.2 (3) |
| O1—C7—C8 | 108.50 (15) | C13—C12—H12A | 115.9 |
| O1—C7—H7A | 110.0 | C2—C12—H12A | 115.9 |
| C8—C7—H7A | 110.0 | C12—C13—C14 | 123.3 (4) |
| O1—C7—H7B | 110.0 | C12—C13—H13A | 118.4 |
| C8—C7—H7B | 110.0 | C14—C13—H13A | 118.4 |
| H7A—C7—H7B | 108.4 | C13—C14—H14A | 109.5 |
| C7—C8—C9 | 111.18 (16) | C13—C14—H14B | 109.5 |
| C7—C8—H8A | 109.4 | H14A—C14—H14B | 109.5 |
| C9—C8—H8A | 109.4 | C13—C14—H14C | 109.5 |
| C7—C8—H8B | 109.4 | H14A—C14—H14C | 109.5 |
| C9—C8—H8B | 109.4 | H14B—C14—H14C | 109.5 |
| H8A—C8—H8B | 108.0 | | |

| | | | |
|---|---|---|---|
| C7—O1—C1—C6 | 3.0 (3) | C2—C1—C6—C5 | 0.7 (3) |
| C7—O1—C1—C2 | −176.00 (16) | C4—C5—C6—C1 | 0.4 (4) |
| O1—C1—C2—C3 | 177.78 (17) | C1—O1—C7—C8 | 177.33 (15) |
| C6—C1—C2—C3 | −1.3 (3) | O1—C7—C8—C9 | −177.21 (15) |
| O1—C1—C2—C12 | −0.6 (3) | C7—C8—C9—C10 | −179.81 (15) |
| C6—C1—C2—C12 | −179.6 (2) | C8—C9—C10—C11 | −176.97 (15) |
| C1—C2—C3—C4 | 0.8 (3) | C9—C10—C11—C11$^{\rm i}$ | 179.19 (18) |
| C12—C2—C3—C4 | 179.1 (2) | C1—C2—C12—C13 | 161.6 (3) |
| C2—C3—C4—C5 | 0.3 (4) | C3—C2—C12—C13 | −16.7 (4) |
| C3—C4—C5—C6 | −0.9 (4) | C2—C12—C13—C14 | 179.0 (3) |
| O1—C1—C6—C5 | −178.27 (19) | | |

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

### *Hydrogen-bond geometry (Å, °)*

Cg1 is the centroid of the C1–C6 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C12—H12···O1 | 0.93 (3) | 2.40 (3) | 2.727 (3) | 101 (3) |
| C7—H7B···Cg1 | 0.97 | 2.65 | 2.396 (3) | 143 |

**Fig. 1**

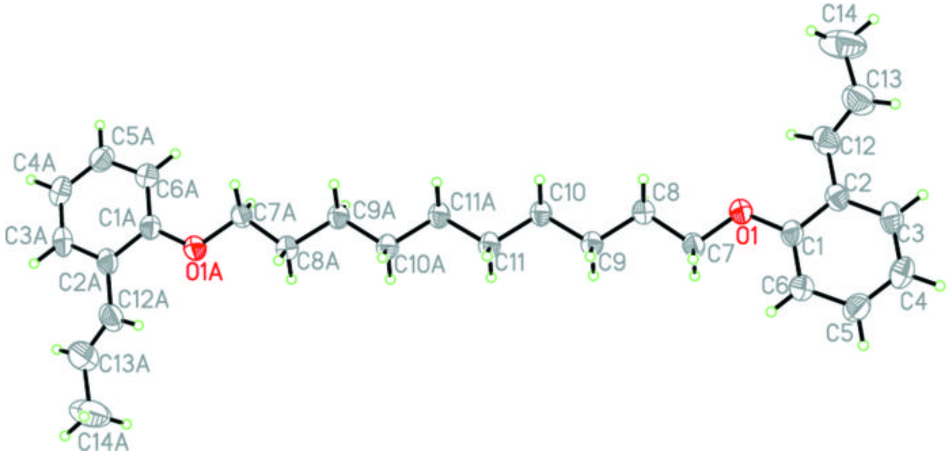
C14
C13
C12
C2
C3
C1
O1
C6
C4
C5
C7
C8
C9
C10
C11
C11A
C10A
C9A
C8A
C7A
O1A
C1A
C6A
C5A
C4A
C3A
C2A
C12A
C13A
C14A

**Fig. 2**