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4,4′-[Isopropylidenebis(*p*-phenyleneoxy)]dibutanoic acid

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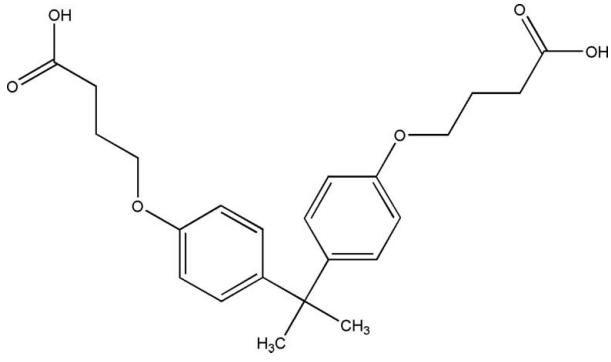
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.122; data-to-parameter ratio = 13.9.

In the title compound, $C_{23}H_{28}O_6$, the mean planes of the two benzene rings make a dihedral angle of 81.1 (2)°. A twofold rotation axis passes through the central C atom. The molecules are connected into chains *via* intermolecular O—H···O hydrogen bonds.

Related literature

For related literature, see: Ferguson *et al.* (1999); Staples *et al.* (1998).



Experimental

Crystal data

$C_{23}H_{28}O_6$
M_r = 400.45
Monoclinic, $C2/c$
a = 17.7714 (6) Å
b = 6.4837 (2) Å
c = 18.9720 (7) Å
β = 103.997 (1)°
V = 2121.13 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (2) K
0.32 × 0.28 × 0.22 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.972, T_{max} = 0.981
11585 measured reflections
1875 independent reflections
1270 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.122
S = 1.04
1875 reflections
135 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.82	1.80	2.615 (2)	170

Symmetry code: (i) $-x, -y, -z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2236).

References

Ferguson, G., Glidewell, C., Gregson, R. M. & Lavender, E. S. (1999). *Acta Cryst.* B**55**, 573–590.
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 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Staples, C. A., Dorn, P. B., Klecka, G. M., O'Block, S. T. & Harris, L. R. (1998). *Chemosphere*, **36**, 2149–2173.

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supplementary materials

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4,4'-[Isopropylidenebis(*p*-phenyleneoxy)]dibutanoic acid

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Comment

Bisphenol A is an intermediate in the production of polycarbonate and epoxy resins, flame retardants, and other specialty products. It is moderately soluble and appears to be released into the environment through its use (Staples *et al.*, 1998). Crystal engineering using bisphenol A derivatives has received attention (Ferguson *et al.*, 1999). In the course of our studies on bisphenol A derivatives, we have synthesized and determined the structure of the title compound (Fig. 1). In the crystal, the mean planes of the two benzene rings make a dihedral angle of 81.1 (2) °. Intermolecular O—H···O hydrogen bonds link the molecules into chains (Fig. 2).

Experimental

To a solution of bisphenol A (0.01 mol) in acetonitrile (50 ml), anhydrous potassium carbonate (0.02 mol) and ethyl 4-bromobutanoate were added (0.01 mol). The solution was refluxed for 6 h and then filtered. The filtrate was evaporated under reduced pressure and the residue was dissolved in water/ethanol (1:2 *v*/*v*), then sodium hydroxide (0.02 mol) was added. The solution was refluxed for 24 h, then acidified with dilute HCl. The crude product that precipitated was filtered off and crystals of the title compound (m.p. 458 K) were obtained by recrystallization from a mixture of water and ethanol (1:1). Elemental analysis calculated: C 68.98, H 7.05%; found: C 68.96, H 7.09%.

Refinement

H atoms were placed in idealized locations with C—H = 0.93—0.97 Å or O—H = 0.82 Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

Figures

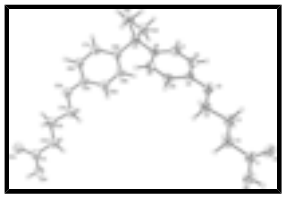


Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level for non-H atoms.

Fig. 2. Detail of (I) showing part of a hydrogen-bonded chain. H atoms have been omitted for clarity and the dashed lines represent the O—H···O hydrogen bonds.

4,4'-[Isopropylidenebis(*p*-phenyleneoxy)]dibutanoic acid

Crystal data

$C_{23}H_{28}O_6$	F_{000} = 856
M_r = 400.45	D_x = 1.254 Mg m^{-3} D_m = 1.254 Mg m^{-3} D_m measured by not measured
Monoclinic, *C*2/*c*	Melting point: 458 K
Hall symbol: -C 2yc	Mo *K*α radiation λ = 0.71073 Å
a = 17.7714 (6) Å	Cell parameters from 1720 reflections
b = 6.4837 (2) Å	θ = 2.4–20.6º
c = 18.9720 (7) Å	μ = 0.09 mm^{-1}
β = 103.997 (1)º	*T* = 295 (2) K
V = 2121.13 (12) Å^3	Block, colourless
Z = 4	0.32 × 0.28 × 0.22 mm

Data collection

Bruker SMART CCD diffractometer	1875 independent reflections
Radiation source: fine-focus sealed tube	1270 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 295(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −20→20
T_{min} = 0.972, T_{max} = 0.981	*k* = −7→7
11585 measured reflections	*l* = −22→20

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.9594P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.122	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.04	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
1875 reflections	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
135 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997a), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0019 (5)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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_{iso}*/U_{eq}
O1	0.03166 (9)	0.2268 (3)	0.03972 (9)	0.0870 (6)
O2	0.09455 (9)	−0.0031 (3)	−0.01063 (10)	0.0840 (5)
H2	0.0521	−0.0601	−0.0193	0.126*
O3	0.23268 (7)	0.7832 (2)	0.13113 (8)	0.0708 (5)
C1	0.09057 (12)	0.1693 (3)	0.02182 (11)	0.0620 (6)
C2	0.16225 (12)	0.2949 (3)	0.03574 (12)	0.0672 (6)
H2A	0.1723	0.3322	−0.0106	0.081*
H2B	0.2051	0.2098	0.0613	0.081*
C3	0.16129 (12)	0.4892 (3)	0.07901 (12)	0.0689 (6)
H3A	0.1208	0.5803	0.0527	0.083*
H3B	0.1497	0.4552	0.1251	0.083*
C4	0.23813 (12)	0.5979 (3)	0.09270 (12)	0.0649 (6)
H4A	0.2786	0.5105	0.1211	0.078*
H4B	0.2509	0.6291	0.0470	0.078*
C5	0.29946 (10)	0.8949 (3)	0.15747 (10)	0.0527 (5)
C6	0.29440 (12)	1.0494 (3)	0.20561 (12)	0.0648 (6)
H6	0.2477	1.0734	0.2181	0.078*
C7	0.35832 (11)	1.1692 (3)	0.23550 (11)	0.0601 (5)
H7	0.3538	1.2729	0.2681	0.072*
C8	0.42893 (10)	1.1398 (3)	0.21848 (10)	0.0493 (5)
C9	0.43194 (11)	0.9847 (3)	0.16914 (11)	0.0606 (6)
H9	0.4784	0.9611	0.1561	0.073*
C10	0.36848 (11)	0.8637 (3)	0.13856 (11)	0.0576 (5)
H10	0.3725	0.7614	0.1053	0.069*
C11	0.5000	1.2749 (4)	0.2500	0.0572 (7)
C12	0.51343 (13)	1.4143 (3)	0.18858 (14)	0.0847 (8)
H12A	0.5272	1.3309	0.1518	0.127*
H12B	0.5547	1.5094	0.2078	0.127*
H12C	0.4668	1.4895	0.1678	0.127*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0724 (10)	0.0757 (11)	0.1180 (14)	−0.0211 (8)	0.0329 (10)	−0.0354 (10)
O2	0.0712 (10)	0.0739 (11)	0.1062 (13)	−0.0166 (8)	0.0202 (9)	−0.0331 (10)
O3	0.0567 (9)	0.0637 (9)	0.0892 (11)	−0.0136 (7)	0.0123 (7)	−0.0165 (8)
C1	0.0641 (13)	0.0555 (13)	0.0629 (13)	−0.0108 (10)	0.0081 (10)	−0.0081 (11)
C2	0.0635 (13)	0.0633 (14)	0.0718 (14)	−0.0130 (10)	0.0103 (11)	−0.0059 (11)
C3	0.0648 (13)	0.0631 (14)	0.0747 (14)	−0.0158 (10)	0.0090 (10)	−0.0088 (11)
C4	0.0659 (13)	0.0552 (13)	0.0690 (13)	−0.0126 (10)	0.0076 (10)	−0.0063 (11)
C5	0.0496 (11)	0.0476 (11)	0.0558 (11)	−0.0034 (9)	0.0029 (9)	0.0008 (9)
C6	0.0544 (12)	0.0660 (14)	0.0764 (14)	−0.0056 (10)	0.0202 (10)	−0.0119 (12)
C7	0.0605 (12)	0.0524 (12)	0.0663 (13)	−0.0005 (9)	0.0133 (10)	−0.0108 (10)
C8	0.0471 (10)	0.0388 (10)	0.0558 (11)	0.0038 (8)	0.0004 (8)	0.0040 (9)
C9	0.0474 (11)	0.0545 (12)	0.0778 (14)	0.0019 (9)	0.0112 (10)	−0.0102 (11)
C10	0.0554 (11)	0.0502 (12)	0.0633 (13)	0.0009 (9)	0.0067 (9)	−0.0110 (10)
C11	0.0531 (15)	0.0379 (15)	0.0730 (19)	0.000	0.0003 (13)	0.000
C12	0.0674 (14)	0.0584 (14)	0.116 (2)	−0.0015 (11)	−0.0012 (13)	0.0348 (14)

Geometric parameters (Å, °)

O1—C1	1.234 (2)	C6—C7	1.380 (3)
O2—C1	1.286 (2)	C6—H6	0.930
O2—H2	0.820	C7—C8	1.383 (3)
O3—C5	1.377 (2)	C7—H7	0.930
O3—C4	1.421 (2)	C8—C9	1.384 (2)
C1—C2	1.481 (3)	C8—C11	1.534 (2)
C2—C3	1.506 (3)	C9—C10	1.381 (3)
C2—H2A	0.970	C9—H9	0.930
C2—H2B	0.970	C10—H10	0.930
C3—C4	1.502 (3)	C11—C8^{i}	1.534 (2)
C3—H3A	0.970	C11—C12^{i}	1.538 (3)
C3—H3B	0.970	C11—C12	1.538 (3)
C4—H4A	0.970	C12—H12A	0.960
C4—H4B	0.970	C12—H12B	0.960
C5—C6	1.373 (3)	C12—H12C	0.960
C5—C10	1.374 (3)		
C1—O2—H2	109.5	C5—C6—H6	119.9
C5—O3—C4	118.11 (15)	C7—C6—H6	119.9
O1—C1—O2	122.88 (19)	C6—C7—C8	122.01 (19)
O1—C1—C2	122.4 (2)	C6—C7—H7	119.0
O2—C1—C2	114.8 (2)	C8—C7—H7	119.0
C1—C2—C3	115.76 (19)	C7—C8—C9	116.36 (17)
C1—C2—H2A	108.3	C7—C8—C11	122.57 (16)
C3—C2—H2A	108.3	C9—C8—C11	121.04 (16)
C1—C2—H2B	108.3	C10—C9—C8	122.40 (18)
C3—C2—H2B	108.3	C10—C9—H9	118.8

H2A—C2—H2B	107.4	C8—C9—H9	118.8
C4—C3—C2	110.92 (18)	C5—C10—C9	119.77 (18)
C4—C3—H3A	109.5	C5—C10—H10	120.1
C2—C3—H3A	109.5	C9—C10—H10	120.1
C4—C3—H3B	109.5	C8—C11—C8^{i}	110.4 (2)
C2—C3—H3B	109.5	C8—C11—C12^{i}	111.51 (11)
H3A—C3—H3B	108.0	C8^{i}—C11—C12^{i}	107.70 (11)
O3—C4—C3	108.26 (17)	C8—C11—C12	107.70 (11)
O3—C4—H4A	110.0	C8^{i}—C11—C12	111.50 (11)
C3—C4—H4A	110.0	C12^{i}—C11—C12	108.0 (3)
O3—C4—H4B	110.0	C11—C12—H12A	109.5
C3—C4—H4B	110.0	C11—C12—H12B	109.5
H4A—C4—H4B	108.4	H12A—C12—H12B	109.5
C6—C5—C10	119.17 (17)	C11—C12—H12C	109.5
C6—C5—O3	115.84 (17)	H12A—C12—H12C	109.5
C10—C5—O3	124.99 (18)	H12B—C12—H12C	109.5
C5—C6—C7	120.29 (18)		
O1—C1—C2—C3	5.1 (3)	C7—C8—C9—C10	−0.5 (3)
O2—C1—C2—C3	−175.24 (19)	C11—C8—C9—C10	−178.49 (18)
C1—C2—C3—C4	177.26 (18)	C6—C5—C10—C9	1.3 (3)
C5—O3—C4—C3	171.96 (17)	O3—C5—C10—C9	−179.46 (18)
C2—C3—C4—O3	177.79 (17)	C8—C9—C10—C5	−0.5 (3)
C4—O3—C5—C6	−167.99 (18)	C7—C8—C11—C8^{i}	130.0 (2)
C4—O3—C5—C10	12.7 (3)	C9—C8—C11—C8^{i}	−52.07 (14)
C10—C5—C6—C7	−1.1 (3)	C7—C8—C11—C12^{i}	10.4 (3)
O3—C5—C6—C7	179.54 (18)	C9—C8—C11—C12^{i}	−171.74 (18)
C5—C6—C7—C8	0.2 (3)	C7—C8—C11—C12	−108.0 (2)
C6—C7—C8—C9	0.6 (3)	C9—C8—C11—C12	69.9 (2)
C6—C7—C8—C11	178.62 (18)		

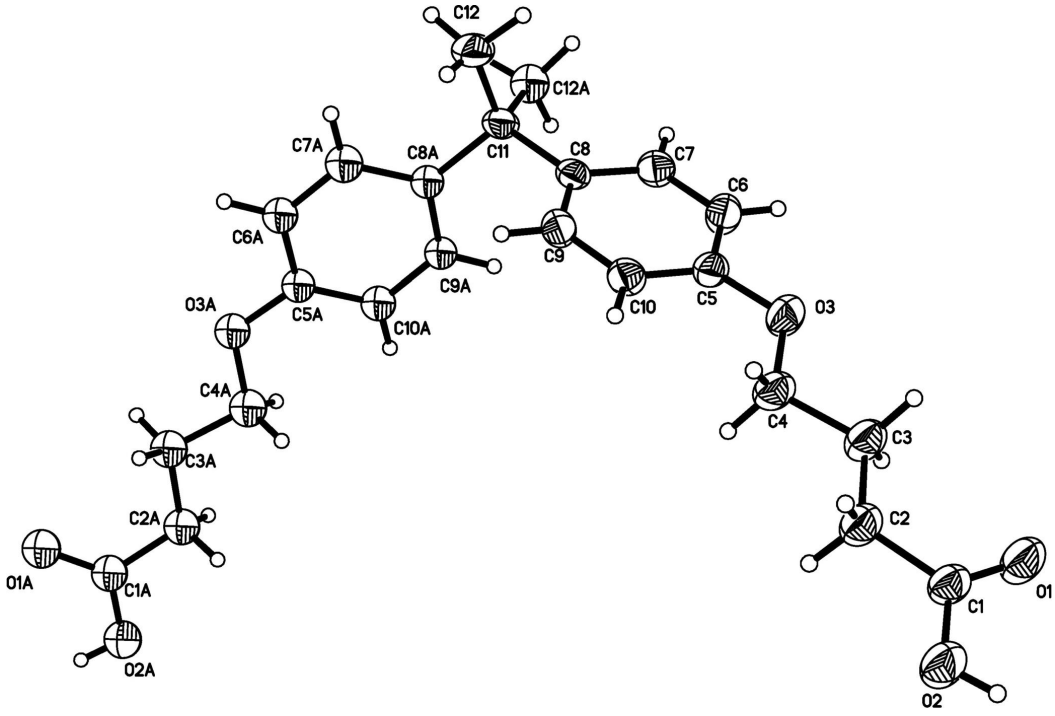
Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{ii}	0.82	1.80	2.615 (2)	170

Symmetry codes: (ii) −*x*, −*y*, −*z*.

Fig. 1


C12
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C11
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C7A
C8
C7
C6
C6A
C9
C9A
C10
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C5A
C10A
C4A
C4
C3
C3A
C2A
C2
O1A
C1A
C1
O1
O2A
O2

Fig. 2