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2-Phenoxyethyl benzoate

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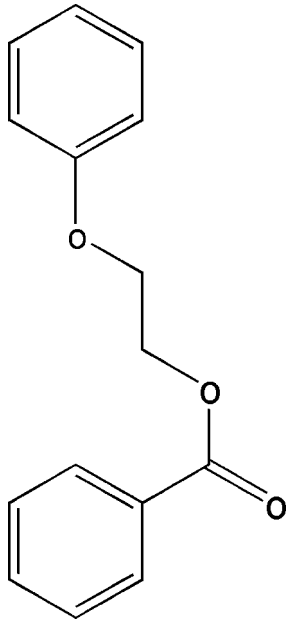
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.130; data-to-parameter ratio = 13.8.

In the title compound, $C_{15}H_{14}O_3$, the dihedral angle between the benzene rings is 75.85 (7)°. In the crystal, centrosymmetrically related molecules are weakly associated through pairs of interactions between a benzene ring and an O atom of the ester group [ring centroid···O = 3.952 (7) Å], and through pairs of interactions between the other benzene ring and an O atom of the phenoxy group [ring centroid···O = 3.912 (7) Å], giving chains extending along [110].

Related literature

For background information and related structures, see: Gandhi *et al.* (1995); Huang *et al.* (1996); Litera *et al.* (2006); Ruzicka *et al.* (2002); Sheehan & Umezaw (1973).



Experimental

Crystal data

$C_{15}H_{14}O_3$
M_r = 242.26
Monoclinic, $P2_1/c$
a = 9.4675 (10) Å
b = 10.1411 (10) Å
c = 13.7792 (12) Å
β = 103.895 (10)°
V = 1284.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.32 × 0.26 × 0.18 mm

Data collection

Oxford Diffraction Xcalibur Eos CCD-detector diffractometer
Absorption correction: analytical (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.995, T_{max} = 0.997
5089 measured reflections
2269 independent reflections
1479 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.130
S = 1.02
2269 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2256).

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supporting information

Acta Cryst. (2013). E**69**, o789 [https://doi.org/10.1107/S1600536813010878]

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Mousa Al-Noaimi, Ismail Warad, Salim F. Haddad, Ahmad Husein and Rami Shareiah

S1. Comment

Phenoxyethyl benzoate has applications in the synthesis of e.g. oxazoles, imidazoles and benzoxazepines (Huang *et al.*, 1996; Gandhi *et al.*, 1995). Esters are also useful as photo-removable protecting groups for carboxylic acids in organic synthesis and biochemistry (Ruzicka *et al.*, 2002; Litera *et al.*, 2006; Sheehan & Umezaw, 1973). Keeping this in view, the title compound, $C_{15}H_{14}O_3$, was synthesized and its crystal structure is repored herein.

In the title compound (Fig. 1), the dihedral angle between the benzene rings is 75.85 (7)°. In the crystal, two centrosymmetrically related molecules are weakly associated through a pair of intermolecular interactions between a benzene ring [C1–C6] and an oxygen of the phenoxy group (O1*A*) [ring centroid(*Cg*)···O1*A* separation, 3.912 (7) Å] [for symmetry code (*A*): -*x*, -*y* + 1, -*z*]. In addition, the molecules are weakly associated through a similar pair of intermolecular interactions between the second benzene ring [C10–C15] and a carboxyl oxygen of the ester group (O2*B*) [ring centroid (*Cg*)···O2*B* separation, 3.952 (7) Å] [for symmetry code (*B*): -*x* + 1, -*y*, -*z*] (Fig. 2). The result is a chain structure extending across [110].

S2. Experimental

Benzoic acid (10.0 g, 0.08 mol) was mixed directly without solvent with 2-phenoxyethanol (11.0 g, 0.08 mol) and refluxed for 3 hours. The reaction was left at room temperature for 24 hours. The product was collected as crystals in 52% yield. The crystals were purified by washing several times with cold ethanol.

S3. Refinement

Hydrogen atoms were positioned geometrically with C—H = 0.93 Å (aromatic) or 0.98 Å (methylene) and allowed to ride in the refinement, with U_{iso}(H) = 1.2U_{eq}(C).

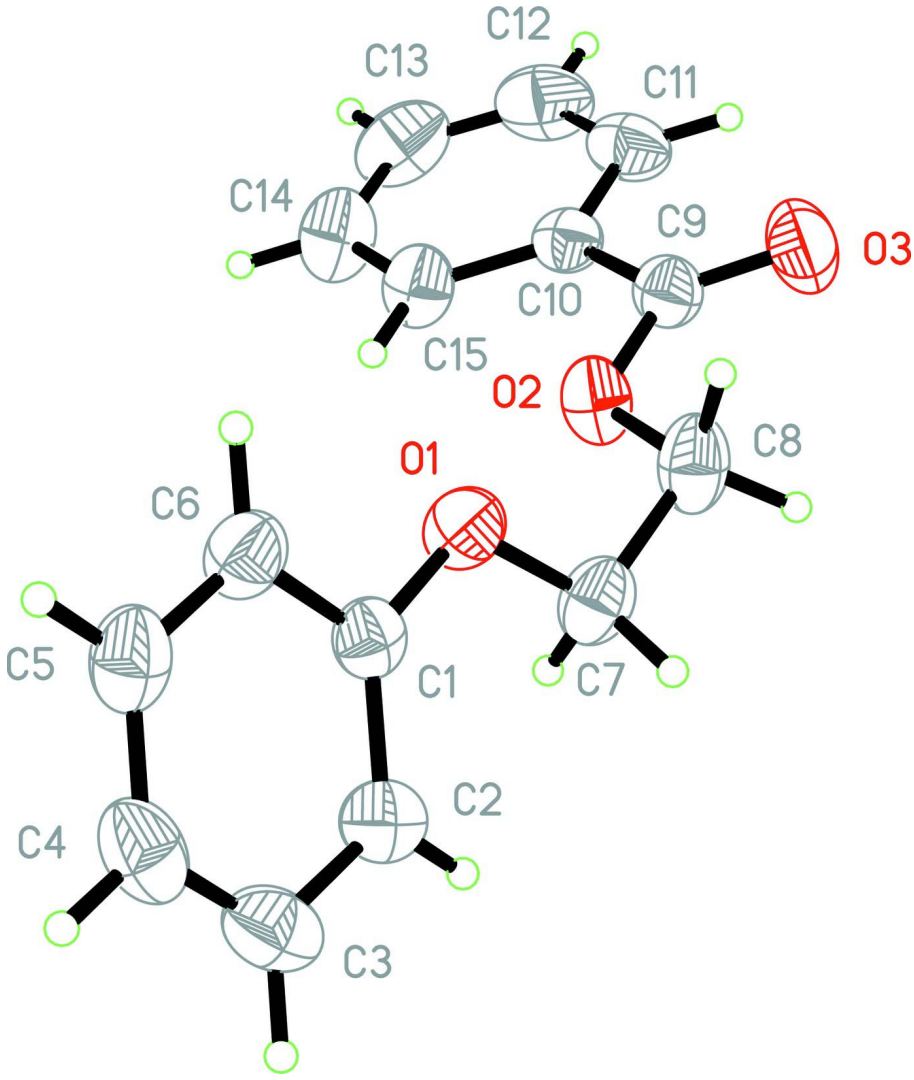

Figure 1

Molecular conformation and atom numbering scheme for the title compound. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms are represented as small spheres of arbitrary radii.

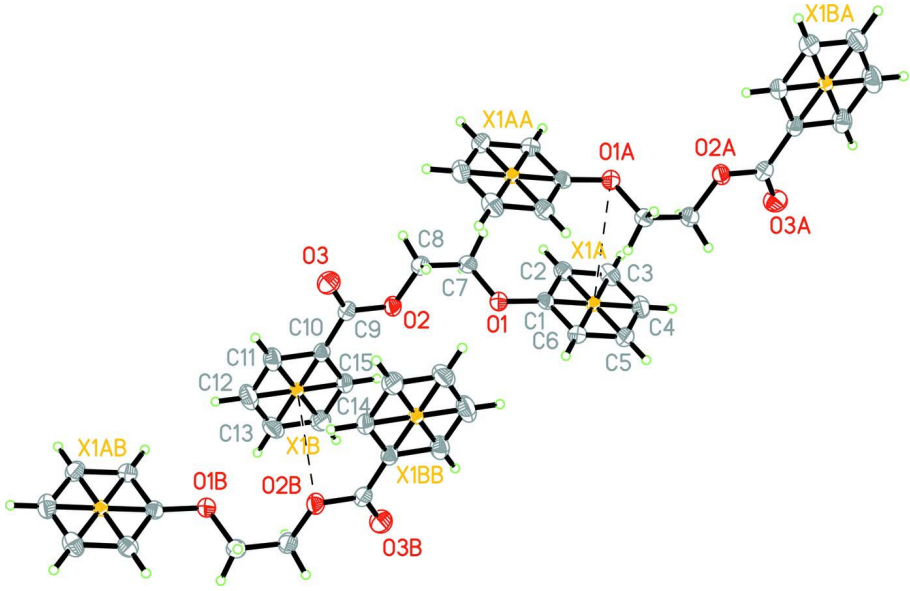

Figure 2

The chain structure showing the ring centroid···O associations [for symmetry code (*A*): -*x*, -*y* + 1, -*z*]; (*B*): -*x* + 1, -*y*, -*z*].

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Crystal data

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$M_r = 242.26$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.4675\ (10)$ Å
$b = 10.1411\ (10)$ Å
$c = 13.7792\ (12)$ Å
$\beta = 103.895\ (10)°$
$V = 1284.2\ (2)$ Å^3
$Z = 4$
$F(000) = 512$
$D_x = 1.253$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1664 reflections
$\theta = 3.0–29.3°$
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Wedge, colourless
0.32 × 0.26 × 0.18 mm

Data collection

Oxford Diffraction Xcalibur Eos CCD-detector diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.0534 pixels mm^{-1}
ω scans
Absorption correction: analytical (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.995$, $T_{max} = 0.997$
5089 measured reflections
2269 independent reflections
1479 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.0°$
$h = -11\rightarrow10$
$k = -9\rightarrow12$
$l = -12\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.130$
$S = 1.02$
2269 reflections
164 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
$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 0.042P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.11$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.035 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.21934 (14)	0.06786 (14)	0.04977 (8)	0.0697 (5)
O1	0.10626 (13)	0.31548 (14)	−0.04881 (9)	0.0693 (4)
C1	0.0173 (2)	0.39845 (19)	−0.11534 (12)	0.0573 (5)
C10	0.37587 (19)	−0.11334 (19)	0.06159 (13)	0.0589 (5)
C9	0.3215 (2)	−0.0031 (2)	0.11219 (14)	0.0644 (5)
C7	0.0433 (2)	0.2408 (2)	0.01671 (14)	0.0703 (6)
H7A	−0.0199	0.1734	−0.0206	0.084*
H7B	−0.0148	0.2977	0.0484	0.084*
C8	0.1615 (2)	0.1781 (2)	0.09424 (14)	0.0786 (6)
H8A	0.2379	0.2417	0.1196	0.094*
H8B	0.1232	0.1479	0.1497	0.094*
O3	0.36163 (17)	0.02131 (18)	0.19998 (10)	0.0968 (6)
C2	−0.1322 (2)	0.4027 (2)	−0.13240 (14)	0.0683 (6)
H2A	−0.1804	0.3477	−0.0970	0.082*
C5	0.0077 (3)	0.5679 (2)	−0.23750 (14)	0.0793 (7)
H5A	0.0554	0.6235	−0.2728	0.095*
C6	0.0870 (2)	0.4820 (2)	−0.16825 (14)	0.0709 (6)
H6A	0.1879	0.4800	−0.1569	0.085*
C11	0.4723 (2)	−0.2012 (2)	0.11906 (17)	0.0810 (7)
H11A	0.5006	−0.1905	0.1881	0.097*
C15	0.3333 (2)	−0.1315 (2)	−0.04026 (15)	0.0737 (6)
H15A	0.2669	−0.0739	−0.0794	0.088*
C3	−0.2097 (2)	0.4898 (2)	−0.20273 (16)	0.0809 (7)
H3A	−0.3107	0.4923	−0.2147	0.097*
C4	−0.1402 (3)	0.5723 (2)	−0.25494 (15)	0.0808 (7)
H4A	−0.1934	0.6307	−0.3018	0.097*
C13	0.4865 (3)	−0.3199 (3)	−0.0267 (2)	0.1029 (8)
H13A	0.5257	−0.3886	−0.0564	0.123*
C14	0.3890 (3)	−0.2350 (2)	−0.08458 (18)	0.0943 (7)

H14A	0.3603	−0.2471	−0.1534	0.113*
C12	0.5261 (3)	−0.3035 (3)	0.0747 (2)	0.1039 (9)
H12A	0.5904	−0.3628	0.1138	0.125*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0937 (10)	0.0559 (9)	0.0580 (7)	0.0144 (8)	0.0151 (7)	0.0017 (7)
O1	0.0707 (8)	0.0666 (9)	0.0747 (8)	0.0111 (7)	0.0255 (7)	0.0141 (7)
C1	0.0673 (12)	0.0505 (12)	0.0551 (10)	0.0079 (10)	0.0163 (9)	−0.0068 (9)
C10	0.0561 (11)	0.0540 (12)	0.0664 (12)	−0.0040 (10)	0.0146 (9)	0.0108 (10)
C9	0.0665 (12)	0.0659 (14)	0.0601 (11)	−0.0028 (11)	0.0139 (9)	0.0091 (11)
C7	0.0862 (14)	0.0593 (14)	0.0730 (12)	0.0087 (12)	0.0342 (10)	0.0017 (11)
C8	0.1139 (17)	0.0638 (14)	0.0627 (11)	0.0174 (13)	0.0303 (12)	0.0018 (11)
O3	0.1082 (12)	0.1176 (15)	0.0581 (8)	0.0162 (10)	0.0073 (8)	−0.0040 (9)
C2	0.0685 (13)	0.0602 (14)	0.0758 (12)	0.0002 (11)	0.0164 (10)	−0.0068 (11)
C5	0.1058 (18)	0.0711 (16)	0.0663 (12)	0.0138 (14)	0.0312 (12)	0.0101 (12)
C6	0.0747 (13)	0.0719 (15)	0.0716 (12)	0.0103 (12)	0.0284 (10)	0.0065 (12)
C11	0.0631 (13)	0.0809 (17)	0.0913 (15)	0.0054 (12)	0.0036 (11)	0.0145 (14)
C15	0.0933 (15)	0.0593 (14)	0.0717 (13)	0.0159 (12)	0.0262 (11)	0.0103 (11)
C3	0.0709 (13)	0.0768 (17)	0.0855 (14)	0.0073 (13)	0.0003 (12)	−0.0152 (14)
C4	0.1031 (18)	0.0686 (16)	0.0614 (12)	0.0196 (14)	0.0018 (12)	−0.0062 (11)
C13	0.107 (2)	0.0694 (17)	0.148 (2)	0.0217 (16)	0.0600 (19)	0.0079 (19)
C14	0.126 (2)	0.0727 (17)	0.0922 (15)	0.0136 (16)	0.0415 (14)	0.0034 (14)
C12	0.0790 (16)	0.089 (2)	0.139 (2)	0.0257 (15)	0.0167 (16)	0.0231 (19)

Geometric parameters (Å, º)

O2—C9	1.339 (2)	C5—C4	1.364 (3)
O2—C8	1.445 (2)	C5—C6	1.374 (3)
O1—C1	1.373 (2)	C5—H5A	0.9300
O1—C7	1.415 (2)	C6—H6A	0.9300
C1—C2	1.379 (2)	C11—C12	1.364 (3)
C1—C6	1.384 (3)	C11—H11A	0.9300
C10—C15	1.376 (2)	C15—C14	1.381 (3)
C10—C11	1.381 (3)	C15—H15A	0.9300
C10—C9	1.474 (3)	C3—C4	1.370 (3)
C9—O3	1.203 (2)	C3—H3A	0.9300
C7—C8	1.491 (3)	C4—H4A	0.9300
C7—H7A	0.9700	C13—C12	1.367 (3)
C7—H7B	0.9700	C13—C14	1.369 (3)
C8—H8A	0.9700	C13—H13A	0.9300
C8—H8B	0.9700	C14—H14A	0.9300
C2—C3	1.384 (3)	C12—H12A	0.9300
C2—H2A	0.9300		
C9—O2—C8	115.63 (14)	C4—C5—H5A	119.7
C1—O1—C7	117.97 (14)	C6—C5—H5A	119.7

O1—C1—C2	124.94 (18)	C5—C6—C1	120.2 (2)
O1—C1—C6	115.68 (17)	C5—C6—H6A	119.9
C2—C1—C6	119.39 (18)	C1—C6—H6A	119.9
C15—C10—C11	119.3 (2)	C12—C11—C10	120.0 (2)
C15—C10—C9	122.27 (17)	C12—C11—H11A	120.0
C11—C10—C9	118.41 (18)	C10—C11—H11A	120.0
O3—C9—O2	122.7 (2)	C10—C15—C14	120.2 (2)
O3—C9—C10	124.74 (18)	C10—C15—H15A	119.9
O2—C9—C10	112.59 (16)	C14—C15—H15A	119.9
O1—C7—C8	109.06 (16)	C4—C3—C2	121.1 (2)
O1—C7—H7A	109.9	C4—C3—H3A	119.5
C8—C7—H7A	109.9	C2—C3—H3A	119.5
O1—C7—H7B	109.9	C5—C4—C3	119.3 (2)
C8—C7—H7B	109.9	C5—C4—H4A	120.3
H7A—C7—H7B	108.3	C3—C4—H4A	120.3
O2—C8—C7	108.78 (15)	C12—C13—C14	120.0 (3)
O2—C8—H8A	109.9	C12—C13—H13A	120.0
C7—C8—H8A	109.9	C14—C13—H13A	120.0
O2—C8—H8B	109.9	C13—C14—C15	119.7 (2)
C7—C8—H8B	109.9	C13—C14—H14A	120.1
H8A—C8—H8B	108.3	C15—C14—H14A	120.1
C1—C2—C3	119.3 (2)	C11—C12—C13	120.7 (2)
C1—C2—H2A	120.3	C11—C12—H12A	119.7
C3—C2—H2A	120.3	C13—C12—H12A	119.7
C4—C5—C6	120.7 (2)		

C7—O1—C1—C2	−8.7 (3)	O1—C1—C6—C5	179.26 (17)
C7—O1—C1—C6	171.67 (16)	C2—C1—C6—C5	−0.3 (3)
C8—O2—C9—O3	1.1 (3)	C15—C10—C11—C12	1.0 (3)
C8—O2—C9—C10	−179.74 (16)	C9—C10—C11—C12	−179.3 (2)
C15—C10—C9—O3	−175.5 (2)	C11—C10—C15—C14	−1.3 (3)
C11—C10—C9—O3	4.7 (3)	C9—C10—C15—C14	178.9 (2)
C15—C10—C9—O2	5.3 (3)	C1—C2—C3—C4	−0.5 (3)
C11—C10—C9—O2	−174.41 (17)	C6—C5—C4—C3	−0.2 (3)
C1—O1—C7—C8	−169.37 (15)	C2—C3—C4—C5	0.3 (3)
C9—O2—C8—C7	−176.41 (17)	C12—C13—C14—C15	1.3 (4)
O1—C7—C8—O2	−75.6 (2)	C10—C15—C14—C13	0.2 (4)
O1—C1—C2—C3	−179.05 (17)	C10—C11—C12—C13	0.5 (4)
C6—C1—C2—C3	0.5 (3)	C14—C13—C12—C11	−1.7 (4)
C4—C5—C6—C1	0.2 (3)		