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4-(4-Propoxybenzoyloxy)benzoic acid

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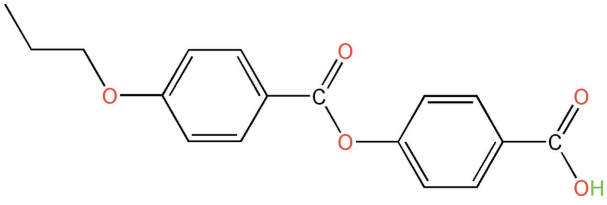
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.004 Å; R factor = 0.085; wR factor = 0.147; data-to-parameter ratio = 16.4.

The title compound, $C_{17}H_{16}O_5$, is an important intermediate for the synthesis of side-chain ligands for polymeric liquid crystals. The propoxy and benzoic acid groups subtend dihedral angles of 4.36 (6) and 55.35 (6)°, respectively, with the central benzoyloxy unit. The crystal structure is stabilized by an intermolecular O—H···O hydrogen bond.

Related literature

For related literature, see: Ahmad *et al.* (2003); Aranzazu *et al.* (2006); Cady *et al.* (2002); Hameed & Rama (2004); Hartung *et al.* (1997); Hussain *et al.* (2003, 2005); Kong & Tang (1998); Nazir *et al.* (2008*a*,*b*); Ribeiro *et al.* (2008); Shafiq *et al.* (2003, 2005); Wu & Hsu (2007); Wu & Lin (2007).



Experimental

Crystal data

$C_{17}H_{16}O_5$
M_r = 300.30
Monoclinic, $C2/c$
a = 21.063 (15) Å
b = 5.703 (4) Å
c = 24.437 (18) Å
β = 99.790 (9)°
V = 2893 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 123 (2) K
0.30 × 0.19 × 0.15 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Absorption correction: empirical (*NUMABS*; Higashi, 1999)
T_{min} = 0.970, T_{max} = 0.985
11426 measured reflections
3297 independent reflections
2824 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.084
$wR(F^2)$ = 0.146
S = 1.26
3297 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3*O*···O4^{i}	0.84	1.77	2.606 (3)	172

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

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97* and *TEXSAN*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2407).

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supplementary materials

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4-(4-Propoxybenzoyloxy)benzoic acid

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Comment

Differently substituted aromatic carboxylic acids having benzene rings either joined directly through a covalent bond (Wu & Hsu 2007) or through some functional group, mostly an ester (Cady *et al.*, 2002; Wu & Lin 2007) or an olefin (Nazir *et al.*, 2008*a*; 2008*b*), have been investigated for their liquid crystal properties. Such acids have been used in the synthesis of intermediates for side-chain liquid crystal polymers (Kong & Tang 1998) as well as for main-chain liquid crystal polymers (Aranzazu *et al.*, 2006). In addition, the carboxylic acids, in general, have been used as intermediates in the synthesis of a large number of organic compounds (Hussain *et al.*, 2005; 2003; Shafiq *et al.*, 2005; 2003; Ahmad *et al.*, 2003). The pharmaceutical industry has also benefited from this class of compounds (Ribeiro *et al.*, 2008; Hameed & Rama, 2004). The title compound (I) was synthesized in our lab as an intermediate in the synthesis of side-chain liquid crystal polymers, by treating 4-hydroxybenzaldehyde with 4-propyloxybenzoylchloride followed by $KMnO_4$ oxidation. In this report, the crystal structure of (I) is presented. Bond lengths and angles are within the normal ranges as given for benzoyloxybenzoic acids (Hartung *et al.*, 1997). The C(14)—O(4), C(14)—O(3),*C*(7)—O(1) and C(7)—O(2) bond lengths are 1.237 (3), 1.300 (3), 1.204 (3) and 1.367 (3) respectively, clearly indicating the partial double bond character of the carboxylate groups. The benzoic acid groups subtend dihedral angles [55.35 (6)°] with the central benzoyloxy moiety C(1)/C(2)/C(3)/C(4)/C(5)/C(6)/C(7)/O(1)/O(2). Two molecules related by an inversion center form a dimer *via* two hydrogen bonds composed of two carboxyl groups as shown in Fig. 2.

Experimental

To a solution of 4-hydroxybenzaldehyde (0.032 moles) in 50 ml of triethylamine (TEA) was added an equivalent amount of 4-propoxybenzoylchloride with stirring and the mixture heated at 333 K for 1 hour. The excess TEA was removed in vacuo and the product, after recrystallization from hot ethanol, was subjected to $KMnO_4$ oxidation. The 4-(4-propoxybenzoyloxy)benzaldehyde (0.025 moles) was dissolved in acetone (100 ml) and aqueous $KMnO_4$ (0.025 moles) was added dropwise at room temperature with stirring. The stirring was continued for three hours when the reaction mixture was filtered and the filtrate acidified using 6M HCl. The product was purified by recrystallization from acetone. Yield: 93% (from 4-(4-propoxybenzoyloxy)benzaldehyde); m.p: 478-480.5K; IR (ν_{max}, KBr, cm^{-1}): 3100-2400, 1731, 1685, 1603, 1512, 1425, 1300, 1260, 1206, 1163, 1061, 1009, 758; ^{1}H-NMR (300 MHz,DMSO-d_6): δ 0.99 (3H, t, J = 7.2 Hz), 1.77 (2H, sex, J = 6.9 Hz), 4.05 (2H, t, J = 6.6 Hz),7.12 (2H, d, J = 8.7 Hz), 7.4 (2H, d, J = 8.7 Hz), 8.03 (2H, d, J = 8.7 Hz),8.08 (2H, d, J = 8.7 Hz), 13.02 (1H, bs); ^{13}C-NMR (75 MHz, DMSO-d_6): 10.75, 22.33, 69.91, 115.16, 120.85, 122.70, 128.79, 131.35, 132.60, 154.65, 163.82, 164.29, 167.12.

Refinement

The O-bound H atom was refined isotropically. All the other H atoms were placed in idealized positions and treated as riding atoms, with C—H distance in the range 0.95–0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C).

Figures

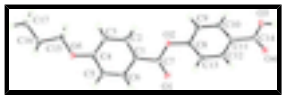

Fig. 1. Molecular structure of (I) showing atom-labelling scheme and displacement ellipsoids at the 30% probability level.

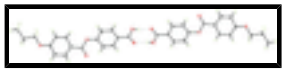

Fig. 2. Showing hydrogen bonded molecules through N—H···O.

4-(4-Propoxybenzoyloxy)benzoic acid

Crystal data

$C_{17}H_{16}O_5$	$F(000) = 1264$
$M_r = 300.30$	$D_x = 1.379$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71070 Å
Hall symbol: -C 2yc	Cell parameters from 3169 reflections
a = 21.063 (15) Å	θ = 3.4–27.5°
b = 5.703 (4) Å	μ = 0.10 mm^{-1}
c = 24.437 (18) Å	*T* = 123 K
β = 99.790 (9)°	Rod, colorless
V = 2893 (3) Å^3	0.30 × 0.19 × 0.15 mm
Z = 8	

Data collection

Rigaku/MSC Mercury CCD diffractometer	3297 independent reflections
Radiation source: fine-focus sealed tube	2824 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.051$
ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
Absorption correction: empirical (using intensity measurements) (*NUMABS*; Higashi, 1999)	*h* = −23→27
$T_{min} = 0.970$, $T_{max} = 0.985$	*k* = −7→5
11426 measured reflections	*l* = −31→31

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.084$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.146$	H-atom parameters constrained
S = 1.26	$w = 1/[\sigma^2(F_o^2) + (0.026P)^2 + 6.5341P]$ where $P = (F_o^2 + 2F_c^2)/3$
3297 reflections	$(\Delta/\sigma)_{max} < 0.001$

201 parameters	$\Delta\rho_{max} = 0.29$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.28$ 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_{iso}*/U_{eq}
C1	0.12026 (11)	0.2626 (4)	0.39828 (9)	0.0171 (5)
C2	0.15716 (12)	0.4515 (4)	0.42065 (10)	0.0223 (5)
H2	0.1686	0.5699	0.3968	0.027*
C3	0.17771 (13)	0.4698 (4)	0.47766 (10)	0.0229 (5)
H3	0.2030	0.6000	0.4926	0.027*
C4	0.16099 (12)	0.2958 (4)	0.51274 (10)	0.0198 (5)
C5	0.12360 (12)	0.1058 (4)	0.49037 (10)	0.0229 (5)
H5	0.1120	−0.0124	0.5142	0.027*
C6	0.10351 (12)	0.0891 (4)	0.43378 (10)	0.0212 (5)
H6	0.0781	−0.0408	0.4188	0.025*
C7	0.09682 (11)	0.2342 (4)	0.33803 (10)	0.0176 (5)
O1	0.06221 (9)	0.0793 (3)	0.31697 (7)	0.0250 (4)
O2	0.11946 (8)	0.4078 (3)	0.30793 (7)	0.0216 (4)
C8	0.09736 (11)	0.4149 (4)	0.25035 (9)	0.0181 (5)
C9	0.06788 (11)	0.6204 (4)	0.22986 (10)	0.0192 (5)
H9	0.0624	0.7460	0.2542	0.023*
C10	0.04640 (11)	0.6402 (4)	0.17308 (10)	0.0177 (5)
H10	0.0254	0.7794	0.1583	0.021*
C11	0.05562 (11)	0.4570 (4)	0.13782 (10)	0.0169 (5)
C12	0.08634 (11)	0.2523 (4)	0.15939 (10)	0.0188 (5)
H12	0.0928	0.1274	0.1352	0.023*
C13	0.10753 (12)	0.2303 (4)	0.21606 (10)	0.0202 (5)
H13	0.1286	0.0915	0.2310	0.024*
C14	0.03310 (11)	0.4762 (4)	0.07712 (10)	0.0177 (5)
O3	0.00181 (9)	0.6673 (3)	0.06089 (7)	0.0272 (4)
H3O	−0.0102	0.6630	0.0263	0.041*
O4	0.04427 (9)	0.3198 (3)	0.04501 (7)	0.0244 (4)
O5	0.17781 (9)	0.2955 (3)	0.56890 (7)	0.0238 (4)
C15	0.21608 (12)	0.4869 (4)	0.59482 (10)	0.0202 (5)
H15A	0.1923	0.6365	0.5875	0.024*

H15B	0.2568	0.4988	0.5799	0.024*
C16	0.22997 (12)	0.4371 (4)	0.65666 (10)	0.0207 (5)
H16A	0.2560	0.2922	0.6636	0.025*
H16B	0.1889	0.4117	0.6704	0.025*
C17	0.26641 (13)	0.6408 (5)	0.68816 (11)	0.0277 (6)
H17A	0.3098	0.6505	0.6788	0.042*
H17B	0.2696	0.6153	0.7282	0.042*
H17C	0.2433	0.7875	0.6777	0.042*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0169 (12)	0.0177 (11)	0.0174 (12)	0.0001 (9)	0.0053 (9)	−0.0012 (9)
C2	0.0269 (13)	0.0199 (12)	0.0207 (13)	−0.0054 (10)	0.0062 (10)	0.0038 (10)
C3	0.0262 (13)	0.0212 (12)	0.0214 (13)	−0.0056 (10)	0.0042 (10)	0.0002 (10)
C4	0.0189 (12)	0.0255 (13)	0.0156 (12)	0.0005 (10)	0.0044 (10)	0.0003 (10)
C5	0.0275 (14)	0.0237 (12)	0.0184 (13)	−0.0057 (10)	0.0061 (10)	0.0025 (10)
C6	0.0220 (13)	0.0210 (12)	0.0213 (13)	−0.0045 (10)	0.0051 (10)	−0.0004 (10)
C7	0.0181 (12)	0.0163 (11)	0.0192 (12)	0.0005 (9)	0.0058 (10)	0.0002 (9)
O1	0.0298 (10)	0.0258 (9)	0.0203 (9)	−0.0100 (8)	0.0067 (8)	−0.0043 (7)
O2	0.0274 (10)	0.0236 (9)	0.0134 (8)	−0.0069 (7)	0.0024 (7)	0.0006 (7)
C8	0.0174 (12)	0.0232 (12)	0.0138 (12)	−0.0057 (9)	0.0031 (9)	0.0022 (9)
C9	0.0193 (12)	0.0188 (11)	0.0203 (12)	−0.0009 (9)	0.0063 (10)	−0.0032 (9)
C10	0.0175 (12)	0.0176 (11)	0.0184 (12)	0.0006 (9)	0.0045 (9)	0.0013 (9)
C11	0.0136 (11)	0.0193 (11)	0.0181 (12)	−0.0008 (9)	0.0040 (9)	0.0014 (9)
C12	0.0204 (12)	0.0173 (11)	0.0198 (12)	−0.0009 (9)	0.0072 (10)	−0.0012 (9)
C13	0.0208 (12)	0.0199 (12)	0.0200 (12)	−0.0007 (9)	0.0036 (10)	0.0021 (9)
C14	0.0153 (11)	0.0190 (11)	0.0196 (12)	0.0013 (9)	0.0055 (9)	−0.0009 (9)
O3	0.0382 (11)	0.0267 (10)	0.0155 (9)	0.0145 (8)	0.0012 (8)	0.0001 (7)
O4	0.0296 (10)	0.0244 (9)	0.0193 (9)	0.0073 (8)	0.0043 (7)	−0.0031 (7)
O5	0.0281 (10)	0.0259 (9)	0.0168 (9)	−0.0071 (8)	0.0024 (7)	0.0004 (7)
C15	0.0200 (12)	0.0220 (12)	0.0184 (12)	−0.0036 (10)	0.0029 (10)	−0.0007 (10)
C16	0.0181 (12)	0.0269 (13)	0.0174 (12)	0.0002 (10)	0.0035 (10)	0.0009 (10)
C17	0.0284 (14)	0.0338 (15)	0.0200 (13)	−0.0014 (11)	0.0012 (11)	0.0000 (11)

Geometric parameters (Å, °)

C1—C2	1.385 (3)	C10—H10	0.9500
C1—C6	1.400 (3)	C11—C12	1.394 (3)
C1—C7	1.480 (3)	C11—C14	1.482 (3)
C2—C3	1.391 (4)	C12—C13	1.387 (3)
C2—H2	0.9500	C12—H12	0.9500
C3—C4	1.395 (3)	C13—H13	0.9500
C3—H3	0.9500	C14—O4	1.237 (3)
C4—O5	1.358 (3)	C14—O3	1.300 (3)
C4—C5	1.395 (3)	O3—H3O	0.8400
C5—C6	1.379 (3)	O5—C15	1.438 (3)
C5—H5	0.9500	C15—C16	1.516 (3)
C6—H6	0.9500	C15—H15A	0.9900

C7—O1	1.204 (3)	C15—H15B	0.9900
C7—O2	1.367 (3)	C16—C17	1.527 (4)
O2—C8	1.406 (3)	C16—H16A	0.9900
C8—C9	1.380 (3)	C16—H16B	0.9900
C8—C13	1.385 (3)	C17—H17A	0.9800
C9—C10	1.389 (3)	C17—H17B	0.9800
C9—H9	0.9500	C17—H17C	0.9800
C10—C11	1.389 (3)		
C2—C1—C6	119.3 (2)	C10—C11—C14	120.7 (2)
C2—C1—C7	123.2 (2)	C12—C11—C14	119.3 (2)
C6—C1—C7	117.6 (2)	C13—C12—C11	120.2 (2)
C1—C2—C3	120.8 (2)	C13—C12—H12	119.9
C1—C2—H2	119.6	C11—C12—H12	119.9
C3—C2—H2	119.6	C8—C13—C12	118.6 (2)
C2—C3—C4	119.6 (2)	C8—C13—H13	120.7
C2—C3—H3	120.2	C12—C13—H13	120.7
C4—C3—H3	120.2	O4—C14—O3	123.5 (2)
O5—C4—C3	124.9 (2)	O4—C14—C11	121.2 (2)
O5—C4—C5	115.3 (2)	O3—C14—C11	115.3 (2)
C3—C4—C5	119.7 (2)	C14—O3—H3O	109.5
C6—C5—C4	120.2 (2)	C4—O5—C15	118.32 (19)
C6—C5—H5	119.9	O5—C15—C16	107.18 (19)
C4—C5—H5	119.9	O5—C15—H15A	110.3
C5—C6—C1	120.4 (2)	C16—C15—H15A	110.3
C5—C6—H6	119.8	O5—C15—H15B	110.3
C1—C6—H6	119.8	C16—C15—H15B	110.3
O1—C7—O2	122.9 (2)	H15A—C15—H15B	108.5
O1—C7—C1	125.5 (2)	C15—C16—C17	110.8 (2)
O2—C7—C1	111.61 (19)	C15—C16—H16A	109.5
C7—O2—C8	118.23 (18)	C17—C16—H16A	109.5
C9—C8—C13	122.2 (2)	C15—C16—H16B	109.5
C9—C8—O2	116.1 (2)	C17—C16—H16B	109.5
C13—C8—O2	121.7 (2)	H16A—C16—H16B	108.1
C8—C9—C10	118.8 (2)	C16—C17—H17A	109.5
C8—C9—H9	120.6	C16—C17—H17B	109.5
C10—C9—H9	120.6	H17A—C17—H17B	109.5
C11—C10—C9	120.2 (2)	C16—C17—H17C	109.5
C11—C10—H10	119.9	H17A—C17—H17C	109.5
C9—C10—H10	119.9	H17B—C17—H17C	109.5
C10—C11—C12	120.0 (2)		
C6—C1—C2—C3	0.2 (4)	C13—C8—C9—C10	1.5 (4)
C7—C1—C2—C3	179.7 (2)	O2—C8—C9—C10	178.5 (2)
C1—C2—C3—C4	0.0 (4)	C8—C9—C10—C11	−1.1 (3)
C2—C3—C4—O5	−179.5 (2)	C9—C10—C11—C12	0.2 (3)
C2—C3—C4—C5	−0.3 (4)	C9—C10—C11—C14	−179.8 (2)
O5—C4—C5—C6	179.7 (2)	C10—C11—C12—C13	0.3 (3)
C3—C4—C5—C6	0.3 (4)	C14—C11—C12—C13	−179.7 (2)
C4—C5—C6—C1	−0.1 (4)	C9—C8—C13—C12	−1.1 (4)

C2—C1—C6—C5	−0.1 (4)	O2—C8—C13—C12	−177.8 (2)
C7—C1—C6—C5	−179.7 (2)	C11—C12—C13—C8	0.2 (4)
C2—C1—C7—O1	−176.3 (2)	C10—C11—C14—O4	175.9 (2)
C6—C1—C7—O1	3.3 (4)	C12—C11—C14—O4	−4.1 (3)
C2—C1—C7—O2	3.8 (3)	C10—C11—C14—O3	−3.7 (3)
C6—C1—C7—O2	−176.6 (2)	C12—C11—C14—O3	176.3 (2)
O1—C7—O2—C8	4.9 (3)	C3—C4—O5—C15	−0.4 (4)
C1—C7—O2—C8	−175.2 (2)	C5—C4—O5—C15	−179.7 (2)
C7—O2—C8—C9	122.6 (2)	C4—O5—C15—C16	−177.7 (2)
C7—O2—C8—C13	−60.5 (3)	O5—C15—C16—C17	−175.9 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3O···O4^{i}	0.84	1.77	2.606 (3)	172.

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

Fig. 1

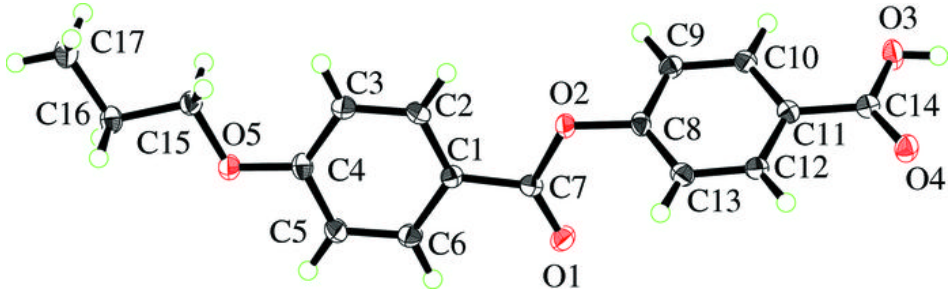
C17
C16
C15
O5
C3
C2
C4
C1
C5
C6
O2
C7
O1
C9
C10
C8
C11
C12
C13
O3
C14
O4

Fig. 2