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2-(*m*-Tolyloxy)benzoic acid

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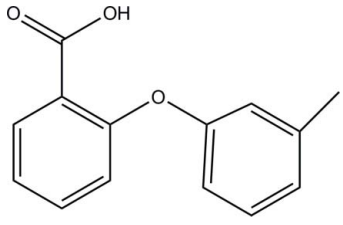
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.052; wR factor = 0.116; data-to-parameter ratio = 13.8.

In the crystal structure of the title compound, $C_{14}H_{12}O_3$, the molecules form classical O—H···O hydrogen-bonded carboxylic acid dimers. The dihedral angle between the two rings is 80.9 (3)°.

Related literature

For related structures, see: Shi *et al.* (2011); Raghunathan *et al.* (1982); Zhang (2011). For the synthesis of the title compound, see: Pellon *et al.* (1995). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{14}H_{12}O_3$
M_r = 228.24
Triclinic, $P\overline{1}$
a = 5.193 (1) Å
b = 7.8000 (16) Å
c = 14.868 (3) Å
α = 94.28 (3)°
β = 97.50 (3)°
γ = 102.54 (3)°
V = 579.5 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.982, T_{max} = 0.991
2387 measured reflections
2132 independent reflections
1132 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.116
S = 1.00
2132 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3B···O2^{i}	0.82	1.83	2.648 (2)	176

Symmetry code: (i) $-x+2, -y+2, -z+2$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5059).

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supporting information

Acta Cryst. (2011). E**67**, o1935 [doi:10.1107/S1600536811026171]

2-(*m*-Tolyloxy)benzoic acid

Zhi-Fang Zhang

S1. Comment

Diphenylethers areuseful as herbicides, ignifuges, antiinflammatories and also as intermediatesin the synthesis of xanthones, *p*-dibenzo-furans, and *p*-dibenzo-dioxines (Pellon, *et al.*, 1995). Knowledge of the crystal structure of such benzoic acid derivatives gives us not only information about nuclearity of the complex molecule, but is important in understanding the behaviour of these compounds with respect to the mechanisms of pharmacological activities and physiological activities. Therefore, we have synthesized the title compound, (I), and report its crystal structure here.

The molecular structure of (I) is shown in Fig. 1, and the intermolecular O—H···O hydrogen bond (Table 1) results in the formation of carboxylic acid dimers (Fig. 2). The bond lengths are within normal ranges (Allen *et al.*, 1987). Similar crystal structure of some compounds have been reported (Shi *et al.*, 2011; Raghunathan *et al.*, 1982; Zhang *et al.*., 2011).

In the molecule of (I), the dihedral angle of the rings(C3—C6) and (C8—C13) is 80.9 (3)°, the molecules were connected together *via* O—H···O intermolecular hydrogen bonds to form dimers, which seems to be very effective in the stabilization of the crystal structure.

S2. Experimental

The title compound, (I), was prepared by the method of Ullmann condensation reaction reported in literature (Pellon *et al.*, 1995). A mixture of 2-chlorobenzoic acid (6.26 g; 0.04 mol), *m*-cresol (8.65 g; 0.08 mol), anhydrous K_2CO_3 (11.04 g; 0.08 mol), pyridine (1.58 g; 0.02 mol), Cu powder (0.2 g) and cuprous iodide (0.2 g) in 25 ml water was kept at reflux for two hours. The mixture was then basified with Na_2CO_3 solution and extracted with diethyl ether. The aqueous solution was acidified with HCl, the precipitated solid was filtered off and disolved in NaOH; the basic solution was filtered (charcoal) and acidified with acetic acid. The 2-(3-tolyloxy)benzoic acid was crystalized from the mixture.

S3. Refinement

H atoms were positioned geometrically and refined as riding groups, with O—H = 0.82 and C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with *U*iso(H) = *xU*eq(C), where *x* = 1.2 for aromatic H, and *x* = 1.5 for other H.

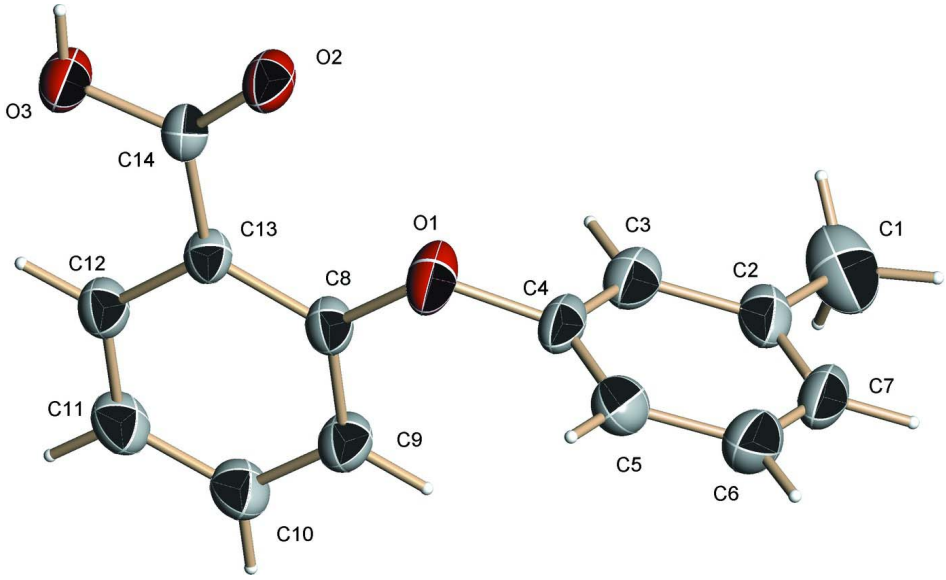

Figure 1

The molecular structure of (I) (thermal ellipsoids are shown at 30% probability levels).

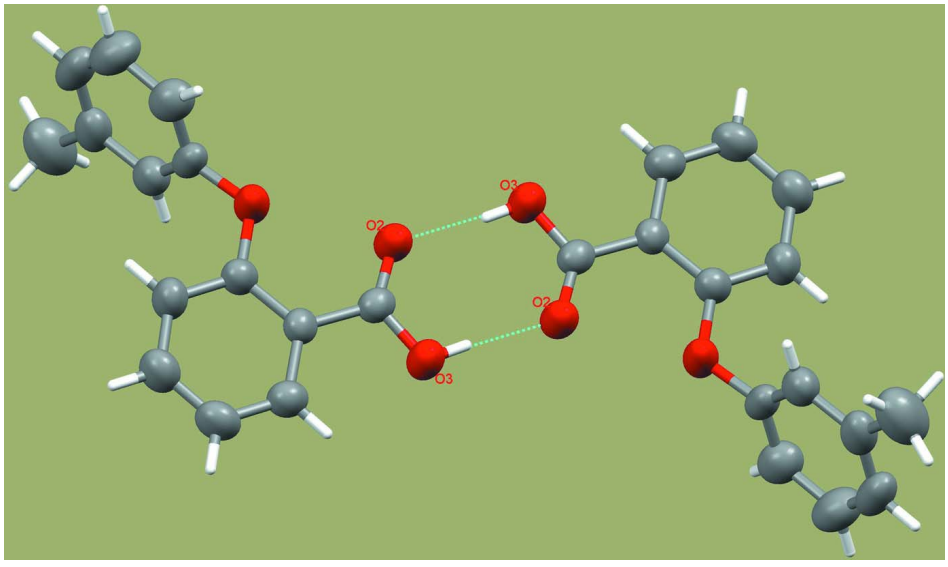

Figure 2

The structure of a dimer of (I).

2-(*m*-Tolyloxy)benzoic acid

Crystal data

$C_{14}H_{12}O_3$
$M_r = 228.24$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.193$ (1) Å
$b = 7.8000$ (16) Å
$c = 14.868$ (3) Å
$\alpha = 94.28$ (3)°
$\beta = 97.50$ (3)°
$\gamma = 102.54$ (3)°
$V = 579.5$ (2) Å^3
$Z = 2$
$F(000) = 240$
$D_x = 1.308$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections

θ = 9–12°
μ = 0.09 mm^{-1}
T = 293 K

Block, colourless
0.20 × 0.20 × 0.10 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} = 0.982, T_{max} = 0.991
2387 measured reflections

2132 independent reflections
1132 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.4°, θ_{min} = 1.4°
h = 0→6
k = −9→9
l = −17→17
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.116
S = 1.00
2132 reflections
155 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
$w = 1/[\sigma^2(F_o^2) + (0.040P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 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}
O1	0.3075 (4)	0.93730 (19)	0.80140 (11)	0.0780 (6)
C1	0.1740 (8)	0.8008 (4)	0.4694 (2)	0.1111 (12)
H1A	0.3613	0.8039	0.4758	0.167*
H1B	0.1429	0.9087	0.4479	0.167*
H1C	0.0778	0.7027	0.4264	0.167*
O2	0.7293 (3)	0.95411 (19)	0.92424 (11)	0.0683 (6)
C2	0.0798 (7)	0.7808 (3)	0.56045 (19)	0.0694 (8)
O3	0.9363 (3)	1.21756 (19)	0.99325 (11)	0.0706 (6)
H3B	1.0355	1.1598	1.0172	0.106*
C3	0.2341 (6)	0.8720 (3)	0.63921 (19)	0.0660 (8)
H3A	0.3994	0.9455	0.6366	0.079*
C4	0.1428 (6)	0.8542 (3)	0.72192 (19)	0.0617 (8)

C5	−0.0968 (6)	0.7484 (3)	0.7283 (2)	0.0720 (8)
H5A	−0.1568	0.7396	0.7844	0.086*
C6	−0.2495 (6)	0.6544 (4)	0.6507 (2)	0.0856 (10)
H6A	−0.4126	0.5789	0.6539	0.103*
C7	−0.1597 (7)	0.6725 (4)	0.5675 (2)	0.0826 (10)
H7A	−0.2652	0.6092	0.5151	0.099*
C8	0.3485 (5)	1.1181 (3)	0.81945 (15)	0.0519 (7)
C9	0.1781 (5)	1.2089 (3)	0.77587 (16)	0.0640 (8)
H9A	0.0352	1.1490	0.7324	0.077*
C10	0.2199 (6)	1.3888 (3)	0.79684 (17)	0.0673 (8)
H10A	0.1049	1.4500	0.7672	0.081*
C11	0.4270 (6)	1.4776 (3)	0.86027 (17)	0.0671 (8)
H11A	0.4544	1.5992	0.8737	0.081*
C12	0.5958 (5)	1.3877 (3)	0.90456 (16)	0.0580 (7)
H12A	0.7366	1.4495	0.9482	0.070*
C13	0.5610 (5)	1.2048 (3)	0.88546 (14)	0.0459 (6)
C14	0.7462 (5)	1.1132 (3)	0.93547 (15)	0.0488 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1006 (15)	0.0443 (9)	0.0743 (12)	0.0174 (10)	−0.0369 (12)	−0.0027 (9)
C1	0.168 (4)	0.092 (2)	0.081 (2)	0.049 (2)	0.014 (2)	0.0103 (19)
O2	0.0736 (13)	0.0455 (9)	0.0766 (12)	0.0160 (9)	−0.0205 (10)	−0.0042 (8)
C2	0.089 (2)	0.0538 (16)	0.0635 (19)	0.0329 (17)	−0.0149 (18)	−0.0047 (14)
O3	0.0756 (13)	0.0522 (10)	0.0735 (12)	0.0157 (10)	−0.0223 (11)	−0.0048 (9)
C3	0.070 (2)	0.0504 (15)	0.0723 (19)	0.0160 (14)	−0.0116 (17)	0.0070 (14)
C4	0.0639 (19)	0.0383 (13)	0.0723 (19)	0.0136 (13)	−0.0245 (16)	−0.0067 (13)
C5	0.070 (2)	0.0588 (16)	0.084 (2)	0.0207 (16)	0.0002 (18)	−0.0067 (15)
C6	0.066 (2)	0.0715 (19)	0.108 (3)	0.0098 (17)	−0.007 (2)	−0.014 (2)
C7	0.081 (2)	0.0577 (17)	0.095 (3)	0.0232 (18)	−0.036 (2)	−0.0216 (17)
C8	0.0642 (17)	0.0412 (12)	0.0474 (14)	0.0131 (13)	−0.0009 (13)	−0.0003 (11)
C9	0.0706 (19)	0.0557 (15)	0.0618 (17)	0.0210 (14)	−0.0129 (15)	0.0011 (13)
C10	0.081 (2)	0.0549 (16)	0.0689 (18)	0.0288 (15)	0.0007 (17)	0.0041 (14)
C11	0.083 (2)	0.0448 (14)	0.0751 (19)	0.0217 (15)	0.0086 (17)	0.0025 (14)
C12	0.0656 (18)	0.0453 (13)	0.0589 (16)	0.0100 (13)	0.0028 (14)	−0.0012 (12)
C13	0.0534 (15)	0.0438 (13)	0.0387 (13)	0.0108 (12)	0.0019 (12)	0.0040 (10)
C14	0.0523 (16)	0.0449 (13)	0.0446 (14)	0.0053 (13)	0.0035 (12)	−0.0012 (11)

Geometric parameters (Å, º)

O1—C8	1.380 (2)	C5—H5A	0.9300
O1—C4	1.389 (3)	C6—C7	1.384 (4)
C1—C2	1.506 (4)	C6—H6A	0.9300
C1—H1A	0.9600	C7—H7A	0.9300
C1—H1B	0.9600	C8—C9	1.377 (3)
C1—H1C	0.9600	C8—C13	1.390 (3)
O2—C14	1.222 (2)	C9—C10	1.378 (3)

C2—C7	1.365 (4)	C9—H9A	0.9300
C2—C3	1.380 (3)	C10—C11	1.357 (3)
O3—C14	1.304 (2)	C10—H10A	0.9300
O3—H3B	0.8200	C11—C12	1.371 (3)
C3—C4	1.380 (3)	C11—H11A	0.9300
C3—H3A	0.9300	C12—C13	1.401 (3)
C4—C5	1.355 (4)	C12—H12A	0.9300
C5—C6	1.371 (3)	C13—C14	1.476 (3)

C8—O1—C4	118.75 (17)	C2—C7—H7A	119.2
C2—C1—H1A	109.5	C6—C7—H7A	119.2
C2—C1—H1B	109.5	C9—C8—O1	121.0 (2)
H1A—C1—H1B	109.5	C9—C8—C13	121.0 (2)
C2—C1—H1C	109.5	O1—C8—C13	118.0 (2)
H1A—C1—H1C	109.5	C8—C9—C10	119.8 (2)
H1B—C1—H1C	109.5	C8—C9—H9A	120.1
C7—C2—C3	118.2 (3)	C10—C9—H9A	120.1
C7—C2—C1	121.2 (3)	C11—C10—C9	120.7 (2)
C3—C2—C1	120.7 (3)	C11—C10—H10A	119.7
C14—O3—H3B	109.5	C9—C10—H10A	119.7
C2—C3—C4	119.9 (3)	C10—C11—C12	119.9 (2)
C2—C3—H3A	120.1	C10—C11—H11A	120.1
C4—C3—H3A	120.1	C12—C11—H11A	120.1
C5—C4—C3	121.6 (3)	C11—C12—C13	121.4 (2)
C5—C4—O1	118.9 (3)	C11—C12—H12A	119.3
C3—C4—O1	119.3 (3)	C13—C12—H12A	119.3
C4—C5—C6	118.9 (3)	C8—C13—C12	117.2 (2)
C4—C5—H5A	120.5	C8—C13—C14	123.17 (19)
C6—C5—H5A	120.5	C12—C13—C14	119.6 (2)
C5—C6—C7	119.7 (3)	O2—C14—O3	121.7 (2)
C5—C6—H6A	120.2	O2—C14—C13	124.1 (2)
C7—C6—H6A	120.2	O3—C14—C13	114.12 (19)
C2—C7—C6	121.7 (3)		

C7—C2—C3—C4	−0.9 (4)	C13—C8—C9—C10	0.9 (4)
C1—C2—C3—C4	179.0 (2)	C8—C9—C10—C11	−0.2 (4)
C2—C3—C4—C5	0.0 (4)	C9—C10—C11—C12	−0.4 (4)
C2—C3—C4—O1	175.7 (2)	C10—C11—C12—C13	0.4 (4)
C8—O1—C4—C5	−110.5 (3)	C9—C8—C13—C12	−0.9 (3)
C8—O1—C4—C3	73.7 (3)	O1—C8—C13—C12	−178.5 (2)
C3—C4—C5—C6	1.3 (4)	C9—C8—C13—C14	178.8 (2)
O1—C4—C5—C6	−174.5 (2)	O1—C8—C13—C14	1.2 (3)
C4—C5—C6—C7	−1.6 (4)	C11—C12—C13—C8	0.2 (4)
C3—C2—C7—C6	0.6 (4)	C11—C12—C13—C14	−179.4 (2)
C1—C2—C7—C6	−179.3 (3)	C8—C13—C14—O2	−0.6 (4)
C5—C6—C7—C2	0.7 (4)	C12—C13—C14—O2	179.0 (2)
C4—O1—C8—C9	18.2 (4)	C8—C13—C14—O3	178.6 (2)
C4—O1—C8—C13	−164.2 (2)	C12—C13—C14—O3	−1.8 (3)

O1—C8—C9—C10	178.4 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*B*···O2^{i}	0.82	1.83	2.648 (2)	176

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