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3,4-Dichlorophenyl benzoate

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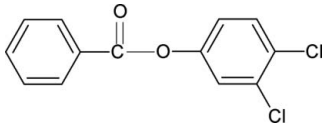
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.116; data-to-parameter ratio = 13.6.

The structure of the title compound, $C_{13}H_8Cl_2O_2$, closely resembles those of phenyl benzoate, 3-methylphenyl benzoate and 4-methylphenyl benzoate, with similar geometric parameters. The dihedral angle between the phenyl and benzoyl rings is 53.77 (5)°, compared to values of 55.7° in phenyl benzoate, 79.61 (6)° in 3-methylphenyl benzoate and 60.17 (7)° in 4-methylphenyl benzoate.

Related literature

For related literature, see: Adams & Morsi (1976); Gowda, Foro, Babitha & Fuess (2007); Gowda, Foro, Nayak & Fuess (2007); Nayak & Gowda (2007).



Experimental

Crystal data

$C_{13}H_8Cl_2O_2$
M_r = 267.09
Monoclinic, $P2_1/c$
a = 6.1145 (7) Å
b = 13.161 (2) Å
c = 14.696 (2) Å
β = 94.20 (1)°
V = 1179.5 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 4.84 mm^{-1}
T = 296 (2) K
0.28 × 0.20 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.350, T_{max} = 0.423
4317 measured reflections
2100 independent reflections
1769 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.116
S = 1.07
2100 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); 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: BT2472).

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supplementary materials

Acta Cryst. (2007). E**63**, o3801 [**doi:10.1107/S1600536807039396**]

3,4-Dichlorophenyl benzoate

B. T. Gowda, S. Foro, K. S. Babitha and H. Fuess

Comment

In the present work, as part of a study of the substituent effects on the structures of chemically and industrially significant compounds (Gowda, Foro, Babitha & Fuess, 2007; Gowda, Foro, Nayak & Fuess, 2007), the structure of 3,4-dichlorophenyl benzoate has been determined. The structure (Fig. 1) is similar to that of phenyl benzoate (Adams & Morsi, 1976), 3-methylphenyl benzoate (Gowda, Foro, Babitha & Fuess, 2007) and 4-methylphenyl benzoate (Gowda, Foro, Nayak & Fuess, 2007). The bond parameters in are similar to those in other benzoates.

Experimental

The title compound was prepared according to a literature method (Nayak & Gowda, 2007). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Nayak & Gowda, 2007). Single crystals of the title compound were obtained by slow evaporation of an ethanolic solution and used for X-ray diffraction studies at room temperature.

Refinement

The H atoms were positioned with idealized geometry using a riding model with C—H = 0.93 Å and with U_{iso}(H) = 1.2 U_{eq} of the parent atom.

Figures

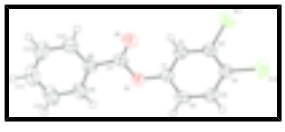

Fig. 1. Molecular structure of the title compound, showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius.

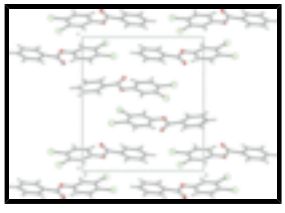

Fig. 2. Packing diagram of the title compound.

3,4-Dichlorophenyl benzoate

Crystal data

$C_{13}H_8Cl_2O_2$	F_{000} = 544
M_r = 267.09	D_x = 1.504 Mg m^{-3}

Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation $\lambda = 1.54180$ Å
Hall symbol: -P 2ybc	Cell parameters from 25 reflections
$a = 6.1145$ (7) Å	$\theta = 3.4$–22.4°
$b = 13.161$ (2) Å	$\mu = 4.84$ mm^{-1}
$c = 14.696$ (2) Å	$T = 296$ (2) K
$\beta = 94.20$ (1)°	Prism, colourless
$V = 1179.5$ (3) Å^3	0.28 × 0.20 × 0.18 mm
$Z = 4$	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.037$
Radiation source: fine-focus sealed tube	$\theta_{max} = 66.9^\circ$
Monochromator: graphite	$\theta_{min} = 4.5^\circ$
$T = 296$(2) K	$h = 0 \rightarrow 7$
$\omega/2\theta$ scans	$k = -15 \rightarrow 12$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = -17 \rightarrow 17$
$T_{min} = 0.350$, $T_{max} = 0.423$	3 standard reflections
4317 measured reflections	every 120 min
2100 independent reflections	intensity decay: 1.0%
1769 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.116$	$w = 1/[\sigma^2(F_o^2) + (0.0717P)^2 + 0.1729P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
2100 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
154 parameters	$\Delta\rho_{min} = -0.42$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$sigma(F^2) is used only for calculat-

ing *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	0.3955 (3)	0.57105 (15)	0.38247 (13)	0.0408 (4)
C2	0.2631 (3)	0.49899 (15)	0.41736 (13)	0.0439 (4)
H2	0.1384	0.5182	0.4457	0.053*
C3	0.3165 (3)	0.39790 (15)	0.40998 (13)	0.0428 (4)
C4	0.5025 (3)	0.36930 (15)	0.36829 (13)	0.0443 (4)
C5	0.6353 (3)	0.44300 (17)	0.33486 (14)	0.0486 (5)
H5	0.7617	0.4241	0.3076	0.058*
C6	0.5829 (3)	0.54449 (17)	0.34145 (13)	0.0466 (5)
H6	0.6723	0.5941	0.3186	0.056*
C7	0.1607 (3)	0.71002 (15)	0.35000 (12)	0.0408 (4)
C8	0.1318 (3)	0.82035 (15)	0.36432 (12)	0.0414 (4)
C9	0.2958 (4)	0.88165 (16)	0.40366 (15)	0.0535 (5)
H9	0.4290	0.8537	0.4257	0.064*
C10	0.2597 (5)	0.98542 (18)	0.40998 (17)	0.0675 (7)
H10	0.3699	1.0273	0.4358	0.081*
C11	0.0625 (5)	1.02650 (18)	0.37843 (17)	0.0688 (7)
H11	0.0392	1.0961	0.3833	0.083*
C12	−0.1004 (4)	0.96541 (19)	0.33972 (17)	0.0650 (6)
H12	−0.2336	0.9938	0.3182	0.078*
C13	−0.0678 (4)	0.86248 (17)	0.33260 (15)	0.0532 (5)
H13	−0.1789	0.8212	0.3066	0.064*
O1	0.3519 (2)	0.67433 (10)	0.39223 (10)	0.0479 (4)
O2	0.0353 (2)	0.65649 (12)	0.30619 (11)	0.0571 (4)
Cl1	0.14815 (11)	0.30812 (4)	0.45478 (5)	0.0679 (2)
Cl2	0.56926 (11)	0.24258 (4)	0.35640 (5)	0.0687 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0372 (9)	0.0385 (9)	0.0461 (10)	−0.0025 (8)	−0.0009 (8)	−0.0036 (8)
C2	0.0391 (10)	0.0449 (10)	0.0488 (10)	−0.0015 (8)	0.0106 (8)	−0.0051 (8)
C3	0.0407 (10)	0.0434 (10)	0.0448 (10)	−0.0065 (8)	0.0062 (8)	−0.0001 (8)
C4	0.0471 (11)	0.0409 (10)	0.0449 (10)	0.0039 (8)	0.0020 (8)	−0.0061 (8)
C5	0.0392 (10)	0.0574 (12)	0.0504 (11)	0.0017 (9)	0.0102 (8)	−0.0048 (9)
C6	0.0364 (9)	0.0520 (11)	0.0518 (11)	−0.0084 (8)	0.0063 (8)	0.0027 (9)
C7	0.0367 (9)	0.0432 (10)	0.0427 (9)	−0.0072 (8)	0.0045 (8)	0.0019 (8)
C8	0.0425 (10)	0.0412 (10)	0.0408 (9)	−0.0034 (8)	0.0050 (8)	0.0054 (7)
C9	0.0576 (12)	0.0445 (11)	0.0565 (12)	−0.0034 (9)	−0.0081 (10)	0.0004 (9)
C10	0.0873 (19)	0.0463 (12)	0.0658 (14)	−0.0084 (12)	−0.0167 (13)	−0.0038 (11)
C11	0.098 (2)	0.0422 (12)	0.0651 (14)	0.0104 (13)	−0.0023 (13)	0.0015 (10)
C12	0.0644 (15)	0.0580 (14)	0.0718 (15)	0.0134 (12)	−0.0003 (12)	0.0115 (11)
C13	0.0455 (11)	0.0518 (12)	0.0621 (13)	−0.0019 (9)	0.0019 (9)	0.0071 (10)

O1	0.0418 (7)	0.0382 (7)	0.0624 (8)	−0.0026 (6)	−0.0054 (6)	−0.0041 (6)
O2	0.0469 (8)	0.0497 (8)	0.0728 (10)	−0.0089 (7)	−0.0076 (7)	−0.0057 (7)
Cl1	0.0676 (4)	0.0481 (3)	0.0911 (5)	−0.0146 (3)	0.0276 (3)	0.0038 (3)
Cl2	0.0754 (4)	0.0474 (3)	0.0844 (4)	0.0121 (3)	0.0138 (3)	−0.0098 (3)

Geometric parameters (Å, °)

C1—C2	1.371 (3)	C7—O1	1.366 (2)
C1—C6	1.378 (3)	C7—C8	1.480 (3)
C1—O1	1.395 (2)	C8—C9	1.380 (3)
C2—C3	1.376 (3)	C8—C13	1.390 (3)
C2—H2	0.9300	C9—C10	1.388 (3)
C3—C4	1.383 (3)	C9—H9	0.9300
C3—Cl1	1.7288 (19)	C10—C11	1.371 (4)
C4—C5	1.379 (3)	C10—H10	0.9300
C4—Cl2	1.729 (2)	C11—C12	1.371 (4)
C5—C6	1.379 (3)	C11—H11	0.9300
C5—H5	0.9300	C12—C13	1.374 (3)
C6—H6	0.9300	C12—H12	0.9300
C7—O2	1.194 (2)	C13—H13	0.9300
C2—C1—C6	121.40 (19)	O1—C7—C8	112.32 (15)
C2—C1—O1	120.86 (17)	C9—C8—C13	120.0 (2)
C6—C1—O1	117.63 (17)	C9—C8—C7	122.87 (19)
C1—C2—C3	119.29 (18)	C13—C8—C7	117.05 (18)
C1—C2—H2	120.4	C8—C9—C10	119.3 (2)
C3—C2—H2	120.4	C8—C9—H9	120.4
C2—C3—C4	120.38 (18)	C10—C9—H9	120.4
C2—C3—Cl1	118.64 (15)	C11—C10—C9	120.4 (2)
C4—C3—Cl1	120.97 (16)	C11—C10—H10	119.8
C5—C4—C3	119.43 (19)	C9—C10—H10	119.8
C5—C4—Cl2	119.55 (16)	C10—C11—C12	120.2 (2)
C3—C4—Cl2	121.01 (16)	C10—C11—H11	119.9
C4—C5—C6	120.70 (19)	C12—C11—H11	119.9
C4—C5—H5	119.7	C11—C12—C13	120.3 (2)
C6—C5—H5	119.7	C11—C12—H12	119.8
C1—C6—C5	118.80 (19)	C13—C12—H12	119.8
C1—C6—H6	120.6	C12—C13—C8	119.8 (2)
C5—C6—H6	120.6	C12—C13—H13	120.1
O2—C7—O1	122.42 (18)	C8—C13—H13	120.1
O2—C7—C8	125.26 (18)	C7—O1—C1	116.90 (14)
C6—C1—C2—C3	−1.0 (3)	O2—C7—C8—C13	7.4 (3)
O1—C1—C2—C3	−177.17 (17)	O1—C7—C8—C13	−173.30 (17)
C1—C2—C3—C4	0.4 (3)	C13—C8—C9—C10	−0.8 (3)
C1—C2—C3—Cl1	179.74 (14)	C7—C8—C9—C10	176.4 (2)
C2—C3—C4—C5	0.6 (3)	C8—C9—C10—C11	0.7 (4)
Cl1—C3—C4—C5	−178.77 (15)	C9—C10—C11—C12	−0.5 (4)
C2—C3—C4—Cl2	−178.71 (15)	C10—C11—C12—C13	0.3 (4)
Cl1—C3—C4—Cl2	1.9 (2)	C11—C12—C13—C8	−0.4 (4)
C3—C4—C5—C6	−0.9 (3)	C9—C8—C13—C12	0.7 (3)

Cl2—C4—C5—C6	178.39 (16)	C7—C8—C13—C12	−176.7 (2)
C2—C1—C6—C5	0.7 (3)	O2—C7—O1—C1	−0.3 (3)
O1—C1—C6—C5	176.96 (17)	C8—C7—O1—C1	−179.62 (16)
C4—C5—C6—C1	0.3 (3)	C2—C1—O1—C7	−64.2 (2)
O2—C7—C8—C9	−169.9 (2)	C6—C1—O1—C7	119.56 (19)
O1—C7—C8—C9	9.4 (3)		

Fig. 1

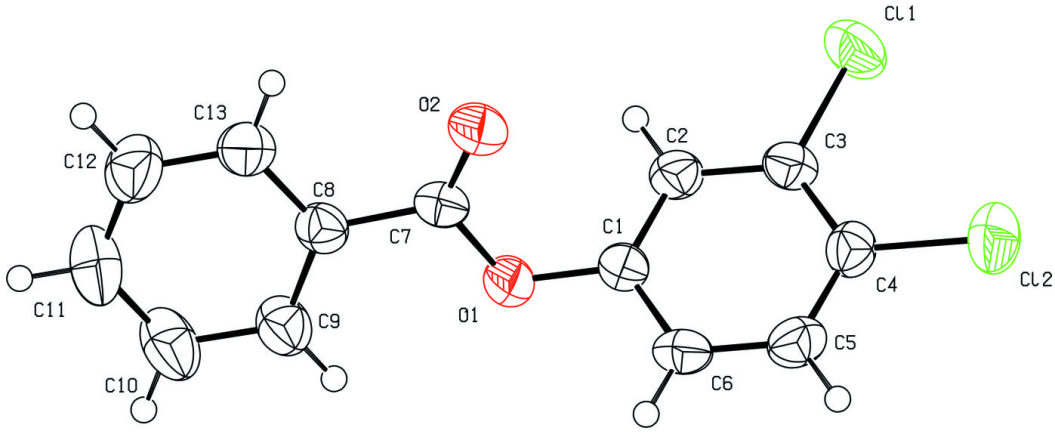

Fig. 2