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2,6-Dichlorophenyl benzoate

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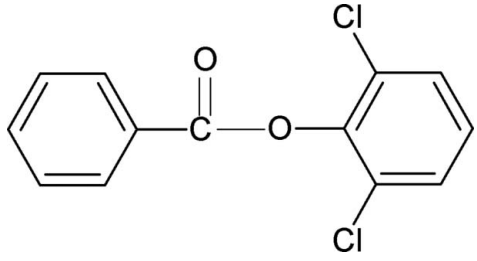
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.005 Å; R factor = 0.049; wR factor = 0.151; data-to-parameter ratio = 14.1.

The structure of the title compound, $C_{13}H_8Cl_2O_2$, is similar to those of phenyl benzoate, 3,4-dichlorophenyl benzoate and other aryl benzoates, with somewhat different bond parameters. The dihedral angle between the two aromatic rings is 75.75 (10)°.

Related literature

For related literature, see: Adams & Morsi (1976); Gowda *et al.* (2007, 2007*a*,*b*); Nayak & Gowda (2007).



Experimental

Crystal data

$C_{13}H_8Cl_2O_2$
M_r = 267.09
Monoclinic, $P2_1/c$
a = 10.500 (2) Å
b = 7.9800 (9) Å
c = 15.007 (2) Å
β = 102.55 (1)°
V = 1227.4 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 4.65 mm^{-1}
T = 299 (2) K
0.55 × 0.35 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.200, T_{max} = 0.406
2541 measured reflections
2185 independent reflections
1553 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
3 standard reflections
frequency: 120 min
intensity decay: 1.5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.151
S = 1.05
2185 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC Software*; 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: BT2486).

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supplementary materials

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2,6-Dichlorophenyl benzoate

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Comment

In the present work, as part of a study of the substituent effects on the structures of chemically and industrially significant compounds (Gowda *et al.*, 2007*a*, *b*; Gowda *et al.*, 2007), the structure of 2,6-dichlorophenyl benzoate (26DCPBA) has been determined. The structure of 26DCPBA (Fig. 1) resembles those of phenyl benzoate (PBA) (Adams & Morsi, 1976), 3,4-dichlorophenyl benzoate (34DCPBA) (Gowda *et al.*, 2007*b*) and other aryl benzoates (Gowda *et al.*, 2007*a*; Gowda *et al.*, 2007). The bond parameters in 26DCPBA are similar to those in PBA, 34DCPBA and other aryl benzoates. The molecules in 26DCPBA are packed into column like structure with the benzoyl ring in the direction of *b* axis, while the dichlorophenyl ring being nearly orthogonal to the former(Fig. 2).

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 (C—H = 0.93 Å) with U_{iso} = 1.2 U_{eq} of the parent atom.

Figures

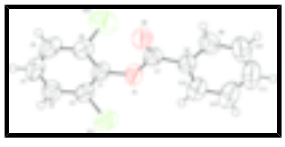

Fig. 1. Molecular structure of the title compound, showing the atom labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius.

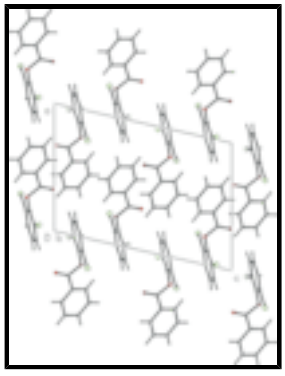

Fig. 2. Molecular packing in the title compound.

2,6-Dichlorophenyl benzoate

Crystal data

$C_{13}H_8Cl_2O_2$	F_{000} = 544
M_r = 267.09	D_x = 1.445 Mg m^{-3}
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation λ = 1.54180 Å
Hall symbol: -P 2ybc	Cell parameters from 25 reflections
a = 10.500 (2) Å	θ = 8.0–19.6º
b = 7.9800 (9) Å	μ = 4.65 mm^{-1}
c = 15.007 (2) Å	T = 299 (2) K
β = 102.55 (1)º	Prism, colourless
V = 1227.4 (3) Å^3	0.55 × 0.35 × 0.20 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.026
Radiation source: fine-focus sealed tube	θ_{max} = 67.0º
Monochromator: graphite	θ_{min} = 4.3º
T = 299(2) K	h = −12→1
ω/2θ scans	k = 0→9
Absorption correction: ψ scan (North *et al.*, 1968)	l = −17→17
T_{min} = 0.200, T_{max} = 0.406	3 standard reflections
2541 measured reflections	every 120 min
2185 independent reflections	intensity decay: 1.5%
1553 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.049	$w = 1/[\sigma^2(F_o^2) + (0.0891P)^2 + 0.1792P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.151	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.05	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
2185 reflections	$\Delta\rho_{min}$ = −0.40 e Å^{-3}
155 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0197 (15)
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 $F^2 > 2\mathrm{sigma}(F^2)$ 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	0.1122 (3)	0.4256 (3)	0.36182 (17)	0.0603 (7)
C2	0.0090 (3)	0.3476 (3)	0.38834 (18)	0.0630 (7)
C3	−0.0996 (3)	0.4377 (4)	0.3971 (2)	0.0719 (8)
H3	−0.1680	0.3846	0.4159	0.086*
C4	−0.1064 (4)	0.6032 (5)	0.3782 (2)	0.0788 (9)
H4	−0.1804	0.6631	0.3834	0.095*
C5	−0.0059 (4)	0.6843 (4)	0.3513 (2)	0.0814 (10)
H5	−0.0117	0.7985	0.3385	0.098*
C6	0.1044 (3)	0.5955 (4)	0.34339 (18)	0.0659 (7)
C7	0.3223 (3)	0.3196 (3)	0.42049 (19)	0.0615 (7)
C8	0.4239 (3)	0.2098 (3)	0.3977 (2)	0.0620 (7)
C9	0.5440 (3)	0.2070 (4)	0.4583 (3)	0.0821 (9)
H9	0.5592	0.2741	0.5101	0.098*
C10	0.6410 (4)	0.1028 (6)	0.4405 (4)	0.1016 (13)
H10	0.7217	0.0989	0.4810	0.122*
C11	0.6184 (4)	0.0059 (6)	0.3637 (4)	0.1099 (15)
H11	0.6843	−0.0628	0.3519	0.132*
C12	0.4996 (5)	0.0090 (5)	0.3041 (3)	0.1052 (13)
H12	0.4849	−0.0577	0.2520	0.126*
C13	0.4015 (4)	0.1111 (4)	0.3212 (2)	0.0805 (9)
H13	0.3205	0.1128	0.2809	0.097*
O1	0.21813 (19)	0.3328 (3)	0.34784 (13)	0.0707 (6)
O2	0.3255 (2)	0.3910 (3)	0.49034 (15)	0.0826 (7)
Cl1	0.01973 (10)	0.13767 (9)	0.41347 (6)	0.0910 (4)
Cl2	0.23311 (11)	0.69468 (14)	0.31154 (7)	0.1058 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0727 (17)	0.0557 (15)	0.0483 (13)	0.0110 (13)	0.0036 (12)	−0.0060 (11)
C2	0.0748 (18)	0.0537 (15)	0.0561 (14)	0.0037 (13)	0.0049 (13)	−0.0045 (12)
C3	0.0705 (18)	0.0787 (19)	0.0643 (16)	0.0103 (16)	0.0096 (14)	−0.0024 (15)

C4	0.087 (2)	0.081 (2)	0.0630 (17)	0.0311 (18)	0.0043 (16)	−0.0047 (15)
C5	0.122 (3)	0.0526 (16)	0.0604 (17)	0.0200 (18)	−0.0015 (18)	0.0003 (13)
C6	0.0821 (19)	0.0575 (16)	0.0537 (15)	0.0021 (14)	0.0053 (13)	0.0015 (12)
C7	0.0679 (17)	0.0553 (14)	0.0600 (16)	0.0013 (12)	0.0109 (13)	0.0013 (12)
C8	0.0642 (16)	0.0517 (14)	0.0720 (17)	0.0043 (12)	0.0187 (14)	0.0128 (12)
C9	0.071 (2)	0.076 (2)	0.097 (2)	0.0011 (16)	0.0145 (17)	0.0142 (18)
C10	0.069 (2)	0.094 (3)	0.146 (4)	0.016 (2)	0.031 (2)	0.035 (3)
C11	0.093 (3)	0.093 (3)	0.159 (4)	0.032 (2)	0.061 (3)	0.030 (3)
C12	0.119 (3)	0.088 (3)	0.120 (3)	0.027 (2)	0.051 (3)	−0.006 (2)
C13	0.085 (2)	0.0741 (19)	0.086 (2)	0.0123 (17)	0.0276 (18)	−0.0015 (17)
O1	0.0699 (12)	0.0779 (13)	0.0614 (11)	0.0193 (10)	0.0079 (9)	−0.0109 (9)
O2	0.0791 (14)	0.0949 (16)	0.0688 (12)	0.0136 (12)	0.0053 (10)	−0.0163 (12)
Cl1	0.1106 (7)	0.0539 (4)	0.1032 (7)	−0.0007 (4)	0.0117 (5)	0.0051 (4)
Cl2	0.1166 (8)	0.1045 (8)	0.0927 (7)	−0.0266 (6)	0.0150 (5)	0.0248 (5)

Geometric parameters (Å, °)

C1—C2	1.380 (4)	C7—O1	1.370 (3)
C1—C6	1.382 (4)	C7—C8	1.478 (4)
C1—O1	1.390 (3)	C8—C13	1.370 (4)
C2—C3	1.378 (4)	C8—C9	1.385 (5)
C2—Cl1	1.715 (3)	C9—C10	1.384 (5)
C3—C4	1.349 (5)	C9—H9	0.9300
C3—H3	0.9300	C10—C11	1.365 (6)
C4—C5	1.371 (5)	C10—H10	0.9300
C4—H4	0.9300	C11—C12	1.369 (7)
C5—C6	1.384 (5)	C11—H11	0.9300
C5—H5	0.9300	C12—C13	1.380 (5)
C6—Cl2	1.721 (3)	C12—H12	0.9300
C7—O2	1.187 (3)	C13—H13	0.9300
C2—C1—C6	118.9 (3)	O1—C7—C8	110.7 (2)
C2—C1—O1	120.5 (3)	C13—C8—C9	120.5 (3)
C6—C1—O1	120.5 (3)	C13—C8—C7	122.3 (3)
C3—C2—C1	120.6 (3)	C9—C8—C7	117.2 (3)
C3—C2—Cl1	120.3 (3)	C10—C9—C8	119.1 (4)
C1—C2—Cl1	119.1 (2)	C10—C9—H9	120.5
C4—C3—C2	119.9 (3)	C8—C9—H9	120.5
C4—C3—H3	120.1	C11—C10—C9	120.2 (4)
C2—C3—H3	120.1	C11—C10—H10	119.9
C3—C4—C5	120.9 (3)	C9—C10—H10	119.9
C3—C4—H4	119.5	C10—C11—C12	120.5 (4)
C5—C4—H4	119.5	C10—C11—H11	119.7
C4—C5—C6	119.7 (3)	C12—C11—H11	119.7
C4—C5—H5	120.2	C11—C12—C13	120.0 (4)
C6—C5—H5	120.2	C11—C12—H12	120.0
C1—C6—C5	120.0 (3)	C13—C12—H12	120.0
C1—C6—Cl2	119.4 (3)	C8—C13—C12	119.7 (4)
C5—C6—Cl2	120.7 (3)	C8—C13—H13	120.1
O2—C7—O1	122.1 (3)	C12—C13—H13	120.1

O2—C7—C8	127.3 (3)	C7—O1—C1	116.6 (2)
C6—C1—C2—C3	−0.5 (4)	O1—C7—C8—C13	−12.2 (4)
O1—C1—C2—C3	−176.2 (2)	O2—C7—C8—C9	−10.0 (4)
C6—C1—C2—Cl1	−178.7 (2)	O1—C7—C8—C9	169.3 (3)
O1—C1—C2—Cl1	5.7 (3)	C13—C8—C9—C10	−0.1 (5)
C1—C2—C3—C4	1.1 (4)	C7—C8—C9—C10	178.5 (3)
Cl1—C2—C3—C4	179.2 (2)	C8—C9—C10—C11	0.7 (5)
C2—C3—C4—C5	−0.8 (5)	C9—C10—C11—C12	−0.7 (6)
C3—C4—C5—C6	0.0 (5)	C10—C11—C12—C13	0.2 (7)
C2—C1—C6—C5	−0.2 (4)	C9—C8—C13—C12	−0.5 (5)
O1—C1—C6—C5	175.4 (2)	C7—C8—C13—C12	−179.0 (3)
C2—C1—C6—Cl2	179.26 (19)	C11—C12—C13—C8	0.4 (6)
O1—C1—C6—Cl2	−5.1 (3)	O2—C7—O1—C1	−4.0 (4)
C4—C5—C6—C1	0.5 (4)	C8—C7—O1—C1	176.6 (2)
C4—C5—C6—Cl2	−179.0 (2)	C2—C1—O1—C7	−93.7 (3)
O2—C7—C8—C13	168.5 (3)	C6—C1—O1—C7	90.7 (3)

Fig. 1

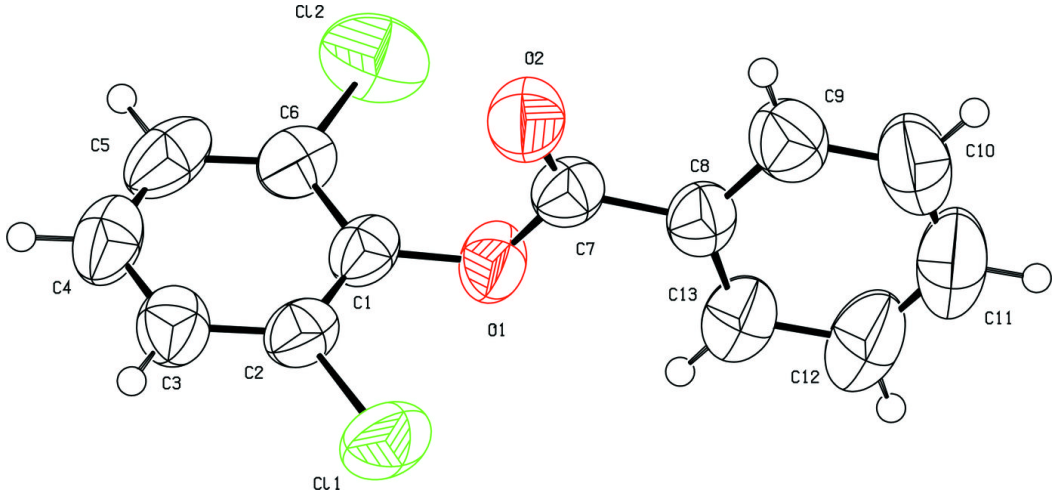

Fig. 2