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2,3-Dichlorophenyl benzoate

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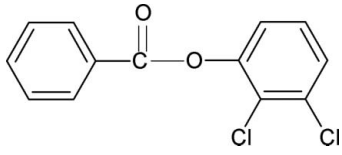
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.129; data-to-parameter ratio = 11.7.

The structure of the title compound (23DCPBA), $C_{13}H_8Cl_2O_2$, resembles that of phenyl benzoate (PBA), 2,6-dichlorophenyl benzoate (26DCPBA) and 3,4-dichlorophenyl benzoate (34DCPBA), with similar geometric parameters. The dihedral angle between the phenyl and benzoyl rings in 23DCPBA is 50.16 (7)°, compared to the value of 55.7° for PBA, 75.75 (10)° for 26DCPBA and 53.77 (5)° for 34DCPBA.

Related literature

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



Experimental

Crystal data

$C_{13}H_8Cl_2O_2$
M_r = 267.09
Monoclinic, $P2_1/c$
a = 10.696 (1) Å
b = 3.9820 (6) Å
c = 27.796 (3) Å
β = 93.045 (8)°
V = 1182.2 (2) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 4.83 mm^{-1}
T = 299 (2) K
0.60 × 0.20 × 0.08 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.370, T_{max} = 0.683
2351 measured reflections
2100 independent reflections
1896 reflections with $I > 2\sigma(I)$
R_{int} = 0.078
3 standard reflections
frequency: 120 min
intensity decay: 0.5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.129
S = 1.08
2100 reflections
179 parameters
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 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: BT2526).

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supplementary materials

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2,3-Dichlorophenyl benzoate

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Comment

In the present work, as part of a study of the substituent effects on the structures of aryl benzoates (Gowda, Foro, Babitha & Fuess, 2007*a*, *b*, *c*; Gowda, Foro, Nayak & Fuess, 2007*a*, Gowda, Foro, Nayak & Fuess, 2007*b*), the structure of 2,3-dichlorophenyl benzoate (23DCPBA) has been determined. The structure of 23DCPBA (Fig. 1) is similar to those of phenyl benzoate (PBA) (Adams & Morsi, 1976); 2,6-dichlorophenyl benzoate (26DCPBA)(Gowda *et al.*, 2007*c*); 3,4-dichlorophenyl benzoate (34DCPBA)(Gowda, Foro, Babitha & Fuess, 2007*b*) and other aryl benzoates (Gowda, Foro, Babitha & Fuess, 2007*a*; Gowda, Foro, Nayak & Fuess, 2007*a*, *b*). The bond parameters in 23DCPBA are similar to those in PBA, 26DCPBA, 34DCPBA and other aryl benzoates. A packing diagram is shown in 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 located in difference map, and their positional parameters were refined with $U_{iso} = 1.2\ U_{eq}$ of the parent atom.

Figures

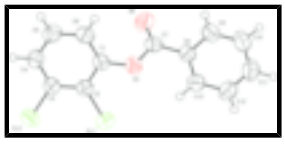

Fig. 1. Molecular structure of the title compound, showing the atom labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius.

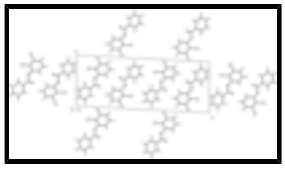

Fig. 2. Packing diagram of the title compound.

2,3-Dichlorophenyl benzoate

Crystal data

$C_{13}H_8Cl_2O_2$ $F_{000} = 544$

M_r = 267.09	D_x = 1.501 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 = 10.696 (1) Å	θ = 5.4–24.7º
b = 3.9820 (6) Å	μ = 4.83 mm^{-1}
c = 27.796 (3) Å	T = 299 (2) K
β = 93.045 (8)º	Thick needle, colourless
V = 1182.2 (2) Å^3	0.60 × 0.20 × 0.08 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.078
Radiation source: fine-focus sealed tube	θ_{max} = 67.0º
Monochromator: graphite	θ_{min} = 3.2º
T = 299(2) K	h = −12→1
ω/2θ scans	k = 0→4
Absorption correction: ψ scan (North *et al.*, 1968)	l = −33→33
T_{min} = 0.370, T_{max} = 0.683	3 standard reflections
2351 measured reflections	every 120 min
2100 independent reflections	intensity decay: 0.5%
1896 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	Only H-atom coordinates refined
$R[F^2 > 2\sigma(F^2)]$ = 0.047	$w = 1/[\sigma^2(F_o^2) + (0.0863P)^2 + 0.2888P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.129	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.08	$\Delta\rho_{max}$ = 0.52 e Å^{-3}
2100 reflections	$\Delta\rho_{min}$ = −0.37 e Å^{-3}
179 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: 0.0027 (6)
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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.35221 (19)	1.1414 (5)	0.33167 (8)	0.0462 (5)
C2	0.25186 (19)	0.9787 (5)	0.35114 (7)	0.0441 (5)
C3	0.15267 (18)	0.8761 (5)	0.32041 (8)	0.0451 (5)
C4	0.1547 (2)	0.9281 (6)	0.27142 (8)	0.0536 (5)
H4	0.088 (3)	0.836 (8)	0.2505 (10)	0.064*
C5	0.2550 (2)	1.0901 (7)	0.25289 (9)	0.0579 (6)
H5	0.251 (3)	1.143 (8)	0.2200 (11)	0.069*
C6	0.3542 (2)	1.1994 (6)	0.28270 (9)	0.0554 (6)
H6	0.414 (3)	1.328 (8)	0.2692 (10)	0.066*
C7	0.5653 (2)	1.1548 (6)	0.35963 (8)	0.0498 (5)
C8	0.6490 (2)	1.2783 (6)	0.39969 (8)	0.0490 (5)
C9	0.7764 (2)	1.2084 (8)	0.39827 (10)	0.0610 (6)
H9	0.804 (3)	1.088 (9)	0.3738 (12)	0.073*
C10	0.8569 (3)	1.3019 (9)	0.43582 (11)	0.0720 (8)
H10	0.948 (3)	1.229 (10)	0.4369 (12)	0.086*
C11	0.8123 (3)	1.4670 (9)	0.47510 (11)	0.0751 (8)
H11	0.868 (3)	1.529 (10)	0.5021 (13)	0.090*
C12	0.6869 (3)	1.5410 (9)	0.47650 (10)	0.0712 (7)
H12	0.659 (3)	1.674 (10)	0.5014 (13)	0.085*
C13	0.6047 (2)	1.4482 (7)	0.43874 (8)	0.0578 (6)
H13	0.516 (3)	1.501 (8)	0.4386 (10)	0.069*
O1	0.44532 (13)	1.2603 (4)	0.36404 (6)	0.0557 (4)
O2	0.59487 (17)	0.9773 (6)	0.32765 (6)	0.0752 (6)
Cl1	0.25156 (6)	0.90985 (17)	0.412174 (18)	0.0618 (2)
Cl2	0.02437 (5)	0.68095 (17)	0.34350 (2)	0.0618 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0443 (10)	0.0418 (11)	0.0526 (11)	0.0037 (8)	0.0033 (9)	−0.0046 (9)
C2	0.0472 (10)	0.0415 (11)	0.0438 (10)	0.0086 (8)	0.0047 (8)	0.0000 (8)
C3	0.0436 (10)	0.0387 (10)	0.0533 (11)	0.0049 (8)	0.0046 (8)	−0.0010 (8)
C4	0.0532 (12)	0.0538 (13)	0.0529 (12)	0.0060 (10)	−0.0066 (10)	0.0007 (10)
C5	0.0636 (14)	0.0612 (14)	0.0489 (12)	0.0071 (11)	0.0028 (10)	0.0110 (10)
C6	0.0550 (12)	0.0514 (13)	0.0604 (13)	−0.0001 (10)	0.0099 (10)	0.0088 (10)
C7	0.0491 (11)	0.0500 (12)	0.0508 (11)	0.0049 (9)	0.0078 (9)	−0.0010 (9)
C8	0.0461 (11)	0.0478 (12)	0.0534 (11)	−0.0029 (9)	0.0057 (9)	0.0041 (9)
C9	0.0503 (12)	0.0706 (16)	0.0623 (13)	0.0026 (11)	0.0055 (11)	0.0028 (12)
C10	0.0508 (13)	0.084 (2)	0.0805 (18)	−0.0093 (13)	−0.0049 (12)	0.0141 (15)

C11	0.0723 (16)	0.088 (2)	0.0636 (14)	−0.0257 (15)	−0.0107 (13)	0.0088 (15)
C12	0.0787 (17)	0.0787 (19)	0.0565 (13)	−0.0171 (15)	0.0057 (12)	−0.0090 (13)
C13	0.0566 (13)	0.0627 (15)	0.0546 (12)	−0.0067 (11)	0.0090 (10)	−0.0047 (11)
O1	0.0433 (8)	0.0604 (10)	0.0634 (9)	0.0013 (7)	0.0028 (7)	−0.0170 (8)
O2	0.0637 (10)	0.0992 (15)	0.0623 (10)	0.0254 (10)	0.0002 (8)	−0.0258 (10)
Cl1	0.0693 (4)	0.0726 (4)	0.0436 (3)	−0.0008 (3)	0.0055 (2)	−0.0013 (2)
Cl2	0.0511 (4)	0.0636 (4)	0.0713 (4)	−0.0080 (2)	0.0106 (3)	−0.0025 (3)

Geometric parameters (Å, °)

C1—C6	1.382 (3)	C7—O1	1.362 (3)
C1—C2	1.388 (3)	C7—C8	1.476 (3)
C1—O1	1.389 (3)	C8—C13	1.384 (3)
C2—C3	1.388 (3)	C8—C9	1.393 (3)
C2—Cl1	1.719 (2)	C9—C10	1.369 (4)
C3—C4	1.379 (3)	C9—H9	0.89 (3)
C3—Cl2	1.730 (2)	C10—C11	1.381 (5)
C4—C5	1.375 (4)	C10—H10	1.02 (3)
C4—H4	0.97 (3)	C11—C12	1.376 (4)
C5—C6	1.381 (4)	C11—H11	0.97 (4)
C5—H5	0.94 (3)	C12—C13	1.383 (4)
C6—H6	0.91 (3)	C12—H12	0.93 (4)
C7—O2	1.192 (3)	C13—H13	0.97 (3)
C6—C1—C2	121.0 (2)	O1—C7—C8	111.49 (18)
C6—C1—O1	122.2 (2)	C13—C8—C9	119.8 (2)
C2—C1—O1	116.67 (19)	C13—C8—C7	122.4 (2)
C3—C2—C1	118.62 (19)	C9—C8—C7	117.9 (2)
C3—C2—Cl1	121.28 (16)	C10—C9—C8	120.1 (3)
C1—C2—Cl1	120.10 (16)	C10—C9—H9	121 (2)
C4—C3—C2	120.8 (2)	C8—C9—H9	119 (2)
C4—C3—Cl2	119.25 (17)	C9—C10—C11	120.1 (3)
C2—C3—Cl2	119.96 (16)	C9—C10—H10	121 (2)
C5—C4—C3	119.6 (2)	C11—C10—H10	119 (2)
C5—C4—H4	121.3 (17)	C12—C11—C10	120.2 (3)
C3—C4—H4	119.0 (17)	C12—C11—H11	119 (2)
C4—C5—C6	120.8 (2)	C10—C11—H11	121 (2)
C4—C5—H5	118.2 (19)	C11—C12—C13	120.2 (3)
C6—C5—H5	120.7 (19)	C11—C12—H12	120 (2)
C5—C6—C1	119.1 (2)	C13—C12—H12	120 (2)
C5—C6—H6	117.4 (18)	C12—C13—C8	119.7 (2)
C1—C6—H6	123.1 (18)	C12—C13—H13	121.8 (18)
O2—C7—O1	122.6 (2)	C8—C13—H13	118.6 (18)
O2—C7—C8	125.9 (2)	C7—O1—C1	118.89 (17)
C6—C1—C2—C3	−0.3 (3)	O1—C7—C8—C13	6.4 (3)
O1—C1—C2—C3	175.68 (18)	O2—C7—C8—C9	6.2 (4)
C6—C1—C2—Cl1	−179.96 (18)	O1—C7—C8—C9	−175.9 (2)
O1—C1—C2—Cl1	−4.0 (3)	C13—C8—C9—C10	1.3 (4)
C1—C2—C3—C4	1.4 (3)	C7—C8—C9—C10	−176.5 (3)
Cl1—C2—C3—C4	−179.01 (17)	C8—C9—C10—C11	−0.3 (5)

C1—C2—C3—Cl2	−178.56 (16)	C9—C10—C11—C12	−0.6 (5)
Cl1—C2—C3—Cl2	1.1 (3)	C10—C11—C12—C13	0.5 (5)
C2—C3—C4—C5	−1.5 (3)	C11—C12—C13—C8	0.5 (4)
Cl2—C3—C4—C5	178.46 (19)	C9—C8—C13—C12	−1.3 (4)
C3—C4—C5—C6	0.5 (4)	C7—C8—C13—C12	176.3 (2)
C4—C5—C6—C1	0.5 (4)	O2—C7—O1—C1	3.8 (4)
C2—C1—C6—C5	−0.6 (4)	C8—C7—O1—C1	−174.26 (19)
O1—C1—C6—C5	−176.4 (2)	C6—C1—O1—C7	−61.0 (3)
O2—C7—C8—C13	−171.5 (3)	C2—C1—O1—C7	123.0 (2)

Fig. 1

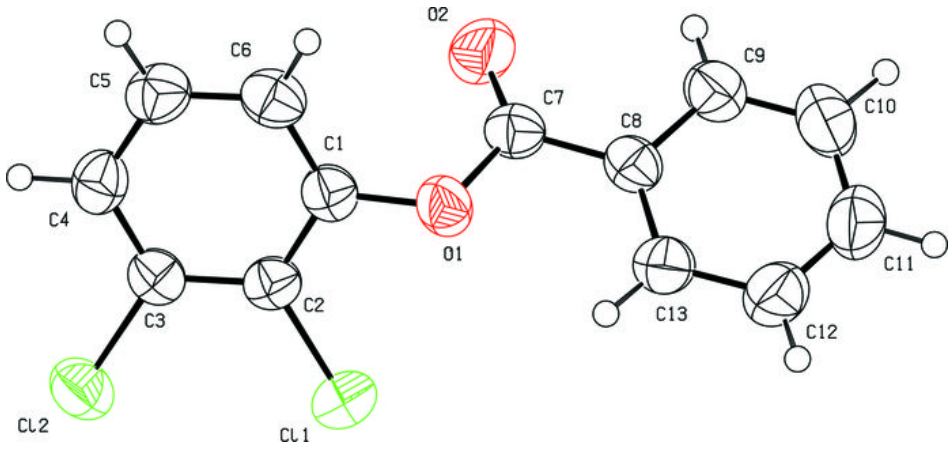

Fig. 2