2,6-Dichlorophenyl 4-methylbenzoate

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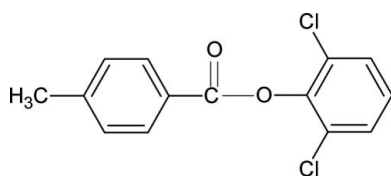
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The structure of the title compound (26DCP4MeBA), $C_{14}H_{10}Cl_2O_2$, resembles those of phenyl benzoate (PBA), 2,6-dichlorophenyl benzoate (26DCPBA), 2,4-dichlorophenyl 4-methylbenzoate (24DCP4MeBA) and other aryl benzoates, with similar bond parameters. The dihedral angle between the benzene and benzoyl rings in 26DCP4MeBA is 77.97 (9)°, compared with values of 55.7 (PBA), 75.75 (10) (26DCPBA) and 48.13 (5)° (24DCP4MeBA). The molecules in the title compound are packed into zigzag chains in the bc plane.

Related literature

For related literature, see: Adams & Morsi (1976); Gowda *et al.* (2007*a*,*b*); Nayak & Gowda (2008).

Experimental

Crystal data

$C_{14}H_{10}Cl_2O_2$	V = 1330.33 (18) Å^3
M_r = 281.12	Z = 4
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation
a = 9.5688 (8) Å	μ = 4.32 mm^{-1}
b = 11.1370 (9) Å	T = 299 (2) K
c = 13.1947 (9) Å	0.60 × 0.35 × 0.30 mm
β = 108.898 (7)°	

Data collection

Enraf–Nonius CAD-4 diffractometer	2366 independent reflections
Absorption correction: ψ scan (North *et al.*, 1968)	2025 reflections with $I > 2\sigma(I)$
T_{min} = 0.202, T_{max} = 0.273	R_{int} = 0.040
3035 measured reflections	3 standard reflections frequency: 120 min intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049	165 parameters
$wR(F^2)$ = 0.168	H-atom parameters constrained
S = 1.01	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
2366 reflections	$\Delta\rho_{min}$ = −0.43 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, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2223).

References

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supporting information

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S1. 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*), the structure of 2,6-dichlorophenyl 4-methylbenzoate (26DCP4MeBA) has been determined. The structure of 26DCP4MeBA (Fig. 1) resembles those of phenyl benzoate (PBA) (Adams & Morsi, 1976), 2,6-dichlorophenyl benzoate (26DCPBA) (Gowda *et al.*, 2007*a*), 2,4-dichlorophenyl 4-methyl benzoate (24DCP4MeBA) (Gowda *et al.*, 2007*b*) and other aryl benzoates. The bond parameters in 26DCP4MeBA are similar to those in PBA, 26DCPBA, 24DCP4MeBA and other benzoates. The dihedral angle between the benzene and benzoyl rings in 26DCP4MeBA is 77.97 (9)°, compared to the values of 55.7° (PBA)(Adams & Morsi, 1976), 75.75 (10)° (26DCPBA) (Gowda *et al.*, 2007*a*) and 48.13 (5)° (24DCP4MeBA)(Gowda *et al.*, 2007*b*). The molecules in 26DCP4MeBA are packed into a zigzag structure with the dichlorophenyl ring being nearly orthogonal to the benzoyl ring (Fig. 2).

S2. Experimental

The title compound was prepared according to a literature method (Nayak & Gowda, 2008). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Nayak & Gowda, 2008). Single crystals of the title compound were obtained by slow evaporation of an ethanolic solution.

S3. Refinement

The H atoms were positioned with idealized geometry using a riding model (C—H = 0.93–0.96 Å) with U_{iso} = 1.2 U_{eq} of the parent atom.
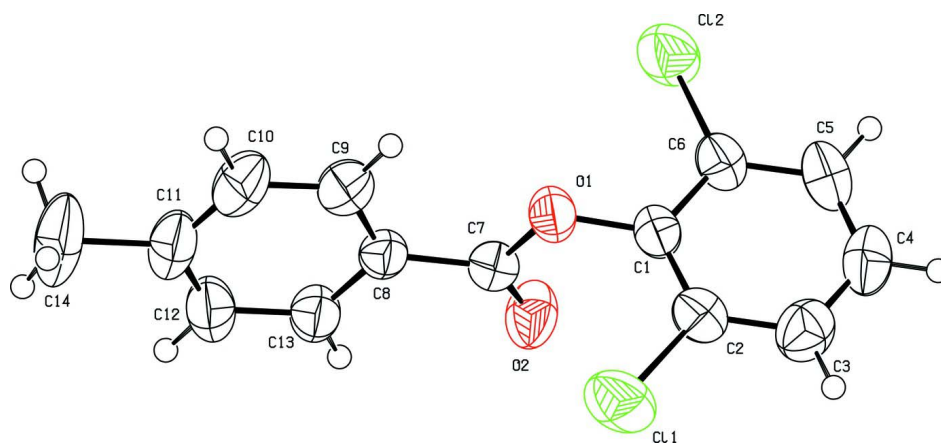

Figure 1

Molecular structure of the title compound, showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level.
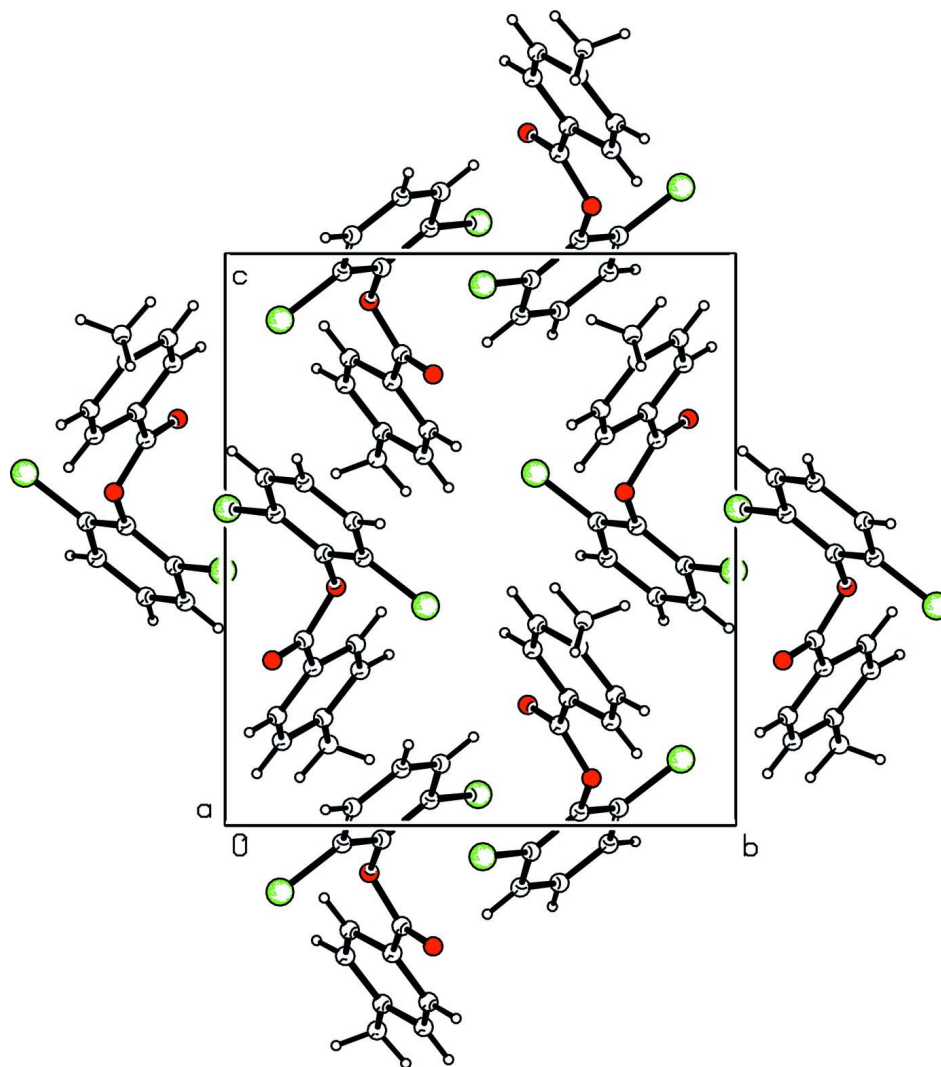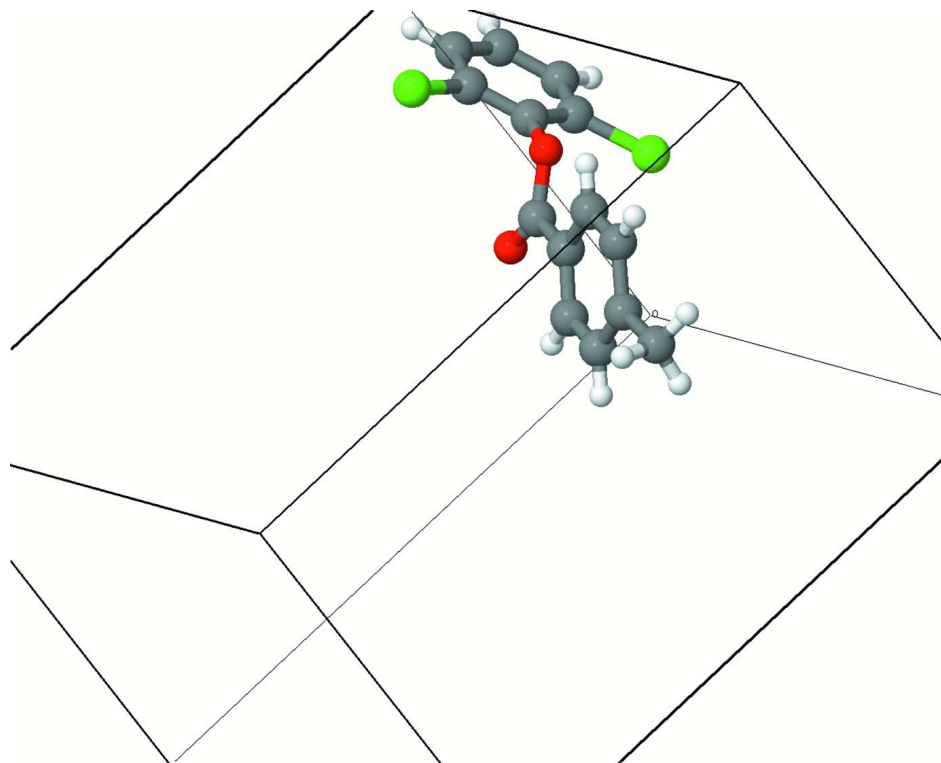
Figure 2

Molecular packing of the title compound as viewed down a.

Figure 3

A view of the title molecule and unit cell

2,6-Dichlorophenyl 4-methylbenzoate

Crystal data

$C_{14}H_{10}Cl_2O_2$

$M_r = 281.12$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 9.5688 (8)$ Å

$b = 11.1370 (9)$ Å

$c = 13.1947 (9)$ Å

$\beta = 108.898 (7)°$

$V = 1330.33 (18)$ Å^3

$Z = 4$

$F(000) = 576$

$D_x = 1.404$ Mg m^{-3}

Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å

Cell parameters from 25 reflections

$\theta = 5.3–18.7°$

$\mu = 4.32$ mm^{-1}

$T = 299$ K

Rod, colourless

$0.60 \times 0.35 \times 0.30$ 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)

$T_{min} = 0.202$, $T_{max} = 0.273$

3035 measured reflections

2366 independent reflections

2025 reflections with $I > 2\sigma(I)$

$R_{int} = 0.040$

$\theta_{max} = 67.0°$, $\theta_{min} = 5.0°$

$h = -11\rightarrow2$

$k = -13\rightarrow0$

$l = -15\rightarrow15$

3 standard reflections every 120 min

intensity decay: none

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.1211P)^2 + 0.3061P]$
$wR(F^2) = 0.168$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.011$
2366 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}
165 parameters	$\Delta\rho_{min} = -0.43$ e Å^{-3}
0 restraints	Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0170 (18)
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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.1987 (2)	0.6943 (2)	0.02446 (17)	0.0490 (5)
C2	0.1627 (3)	0.5987 (2)	−0.0454 (2)	0.0568 (6)
C3	0.0175 (3)	0.5780 (3)	−0.1077 (2)	0.0683 (7)
H3	−0.0065	0.5127	−0.1541	0.082*
C4	−0.0902 (3)	0.6551 (3)	−0.0999 (2)	0.0705 (7)
H4	−0.1879	0.6418	−0.1415	0.085*
C5	−0.0563 (3)	0.7510 (3)	−0.0320 (2)	0.0679 (7)
H5	−0.1304	0.8030	−0.0280	0.082*
C6	0.0887 (3)	0.7707 (2)	0.03086 (19)	0.0547 (6)
C7	0.4023 (2)	0.6546 (2)	0.17553 (18)	0.0499 (5)
C8	0.5626 (2)	0.6726 (2)	0.22269 (17)	0.0484 (5)
C9	0.6386 (3)	0.7563 (2)	0.1830 (2)	0.0636 (7)
H9	0.5881	0.8063	0.1266	0.076*
C10	0.7903 (3)	0.7648 (3)	0.2280 (3)	0.0744 (8)
H10	0.8409	0.8210	0.2009	0.089*
C11	0.8687 (3)	0.6923 (3)	0.3118 (2)	0.0693 (8)
C12	0.7918 (3)	0.6113 (3)	0.3517 (2)	0.0681 (7)
H12	0.8426	0.5620	0.4086	0.082*
C13	0.6393 (3)	0.6016 (2)	0.3082 (2)	0.0574 (6)
H13	0.5887	0.5471	0.3369	0.069*
C14	1.0350 (3)	0.7024 (4)	0.3581 (3)	0.1081 (14)
H14A	1.0606	0.7552	0.4189	0.130*
H14B	1.0733	0.7342	0.3047	0.130*

H14C	1.0766	0.6245	0.3799	0.130*
O1	0.34465 (16)	0.71769 (15)	0.08263 (13)	0.0551 (5)
O2	0.32703 (19)	0.59229 (19)	0.21108 (15)	0.0692 (6)
Cl1	0.30058 (9)	0.50474 (7)	−0.05432 (7)	0.0849 (4)
Cl2	0.13347 (8)	0.89253 (7)	0.11604 (6)	0.0796 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0404 (11)	0.0544 (12)	0.0506 (12)	0.0032 (9)	0.0127 (9)	0.0059 (9)
C2	0.0570 (14)	0.0574 (14)	0.0578 (13)	0.0078 (10)	0.0210 (11)	0.0025 (10)
C3	0.0700 (16)	0.0723 (17)	0.0568 (14)	−0.0073 (13)	0.0124 (12)	−0.0048 (12)
C4	0.0492 (13)	0.093 (2)	0.0597 (15)	−0.0064 (13)	0.0040 (11)	0.0035 (14)
C5	0.0443 (12)	0.091 (2)	0.0654 (15)	0.0142 (12)	0.0139 (11)	0.0084 (14)
C6	0.0488 (12)	0.0627 (14)	0.0522 (12)	0.0091 (10)	0.0157 (10)	0.0002 (10)
C7	0.0464 (12)	0.0493 (12)	0.0528 (12)	−0.0002 (9)	0.0143 (9)	0.0007 (9)
C8	0.0424 (11)	0.0485 (12)	0.0538 (12)	−0.0010 (9)	0.0148 (9)	−0.0070 (9)
C9	0.0577 (14)	0.0586 (14)	0.0741 (16)	−0.0067 (11)	0.0206 (12)	0.0040 (12)
C10	0.0577 (15)	0.0775 (19)	0.090 (2)	−0.0224 (13)	0.0267 (14)	−0.0050 (15)
C11	0.0432 (13)	0.091 (2)	0.0695 (16)	−0.0092 (12)	0.0131 (11)	−0.0208 (14)
C12	0.0478 (13)	0.0830 (18)	0.0635 (15)	0.0035 (12)	0.0042 (11)	−0.0020 (13)
C13	0.0479 (13)	0.0621 (14)	0.0597 (14)	−0.0038 (10)	0.0139 (10)	−0.0018 (10)
C14	0.0438 (15)	0.161 (4)	0.110 (3)	−0.0203 (19)	0.0125 (16)	−0.025 (3)
O1	0.0408 (8)	0.0593 (10)	0.0611 (10)	0.0006 (6)	0.0109 (7)	0.0097 (7)
O2	0.0502 (9)	0.0845 (13)	0.0681 (11)	−0.0149 (8)	0.0125 (8)	0.0170 (9)
Cl1	0.0880 (6)	0.0766 (5)	0.0967 (6)	0.0244 (4)	0.0389 (5)	−0.0084 (4)
Cl2	0.0782 (5)	0.0754 (5)	0.0764 (5)	0.0184 (3)	0.0128 (4)	−0.0178 (3)

Geometric parameters (Å, º)

C1—C6	1.377 (3)	C8—C13	1.379 (3)
C1—C2	1.377 (3)	C8—C9	1.385 (3)
C1—O1	1.383 (3)	C9—C10	1.382 (4)
C2—C3	1.386 (4)	C9—H9	0.9300
C2—Cl1	1.718 (2)	C10—C11	1.379 (4)
C3—C4	1.371 (4)	C10—H10	0.9300
C3—H3	0.9300	C11—C12	1.372 (4)
C4—C5	1.364 (4)	C11—C14	1.513 (4)
C4—H4	0.9300	C12—C13	1.389 (4)
C5—C6	1.384 (4)	C12—H12	0.9300
C5—H5	0.9300	C13—H13	0.9300
C6—Cl2	1.725 (3)	C14—H14A	0.9600
C7—O2	1.199 (3)	C14—H14B	0.9600
C7—O1	1.365 (3)	C14—H14C	0.9600
C7—C8	1.470 (3)		
C6—C1—C2	119.2 (2)	C9—C8—C7	122.4 (2)
C6—C1—O1	120.3 (2)	C10—C9—C8	119.4 (3)

C2—C1—O1	120.4 (2)	C10—C9—H9	120.3
C1—C2—C3	120.8 (2)	C8—C9—H9	120.3
C1—C2—Cl1	119.07 (19)	C11—C10—C9	121.8 (3)
C3—C2—Cl1	120.2 (2)	C11—C10—H10	119.1
C4—C3—C2	119.0 (3)	C9—C10—H10	119.1
C4—C3—H3	120.5	C12—C11—C10	118.2 (2)
C2—C3—H3	120.5	C12—C11—C14	121.3 (3)
C5—C4—C3	121.0 (2)	C10—C11—C14	120.5 (3)
C5—C4—H4	119.5	C11—C12—C13	121.0 (3)
C3—C4—H4	119.5	C11—C12—H12	119.5
C4—C5—C6	119.7 (2)	C13—C12—H12	119.5
C4—C5—H5	120.1	C8—C13—C12	120.2 (2)
C6—C5—H5	120.1	C8—C13—H13	119.9
C1—C6—C5	120.2 (2)	C12—C13—H13	119.9
C1—C6—Cl2	119.48 (19)	C11—C14—H14A	109.5
C5—C6—Cl2	120.26 (19)	C11—C14—H14B	109.5
O2—C7—O1	122.0 (2)	H14A—C14—H14B	109.5
O2—C7—C8	126.1 (2)	C11—C14—H14C	109.5
O1—C7—C8	111.85 (18)	H14A—C14—H14C	109.5
C13—C8—C9	119.3 (2)	H14B—C14—H14C	109.5
C13—C8—C7	118.3 (2)	C7—O1—C1	116.30 (17)
C6—C1—C2—C3	−0.9 (4)	O2—C7—C8—C9	−172.7 (3)
O1—C1—C2—C3	−177.0 (2)	O1—C7—C8—C9	7.8 (3)
C6—C1—C2—Cl1	179.23 (18)	C13—C8—C9—C10	1.7 (4)
O1—C1—C2—Cl1	3.2 (3)	C7—C8—C9—C10	−177.0 (2)
C1—C2—C3—C4	0.8 (4)	C8—C9—C10—C11	−0.2 (5)
Cl1—C2—C3—C4	−179.3 (2)	C9—C10—C11—C12	−1.0 (5)
C2—C3—C4—C5	−0.1 (4)	C9—C10—C11—C14	179.0 (3)
C3—C4—C5—C6	−0.6 (4)	C10—C11—C12—C13	0.5 (4)
C2—C1—C6—C5	0.2 (4)	C14—C11—C12—C13	−179.4 (3)
O1—C1—C6—C5	176.3 (2)	C9—C8—C13—C12	−2.2 (4)
C2—C1—C6—Cl2	−178.59 (18)	C7—C8—C13—C12	176.6 (2)
O1—C1—C6—Cl2	−2.5 (3)	C11—C12—C13—C8	1.0 (4)
C4—C5—C6—C1	0.5 (4)	O2—C7—O1—C1	−8.0 (3)
C4—C5—C6—Cl2	179.3 (2)	C8—C7—O1—C1	171.58 (18)
O2—C7—C8—C13	8.5 (4)	C6—C1—O1—C7	100.0 (3)
O1—C7—C8—C13	−171.0 (2)	C2—C1—O1—C7	−84.0 (3)