organic compounds

2-Methylphenyl 4-methylbenzoate

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The conformation of the C=O bond in the title compound 2MP4MBA, $C_{15}H_{14}O_2$, is *anti* to the *ortho*-methyl group in the phenoxy ring. The bond parameters in 2MP4MBA are similar to those in 3-methylphenyl 4-methylbenzoate (3MP4MBA), 4-methylphenyl 4-methylbenzoate (4MP4MBA) and other aryl benzoates. The dihedral angle between the two aromatic rings in 2MP4MBA is 73.04 (8)°.

Related literature

For related literature, see Gowda *et al.* (2007, 2008); Nayak & Gowda (2008).
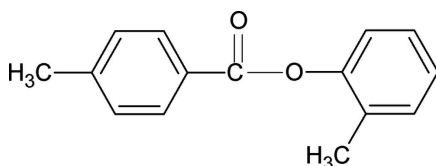
Experimental

Crystal data

$C_{15}H_{14}O_2$
$M_r = 226.26$
Monoclinic, $P2_1/c$
$a = 11.690$ (2) Å
$b = 9.670$ (1) Å
$c = 11.478$ (2) Å
$\beta = 104.50$ (2)°

$V = 1256.2$ (3) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 299$ (2) K
$0.50 \times 0.46 \times 0.20$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford

Diffraction, 2007)
$T_{min} = 0.968$, $T_{max} = 0.989$
7861 measured reflections
2529 independent reflections
1385 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.200$
$S = 1.04$
2529 reflections
181 parameters

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; 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*.

References

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Nayak, R. & Gowda, B. T. (2008). *Z. Naturforsch. Teil A*, **63**. In the press.
Oxford Diffraction (2007). *CrysAlis CCD and CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supporting information

2-Methylphenyl 4-methylbenzoate

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S1. Comment

In the present work, as part of a study of the substituent effects on the crystal structures of aryl benzoates (Gowda *et al.*, 2007; 2008), the structure of 2-methylphenyl 4-methylbenzoate (2MP4MBA) has been determined. The conformation of the C=O bond in 2MP4MBA is *anti* to the *ortho*-methyl group in the phenolic benzene ring (Fig. 1). The bond parameters in 2MP4MBA are similar to those in 3-methylphenyl 4-methylbenzoate (3MP4MBA), 4-methylphenyl 4-methylbenzoate (4MP4MBA) (Gowda *et al.*, 2007) and other aryl benzoates (Gowda *et al.*, 2008). The dihedral angle between the benzene and benzoyl rings in 2MP4MBA is 73.04 (8)°, compared to the values of 56.82 (7)° in 3MP4MBA and 63.57 (5)° in 4MP4MBA. The packing diagram of molecules in the crystal structure is shown in 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 used for X-ray diffraction studies were obtained by slow evaporation of an ethanolic solution at room temperature.

S3. Refinement

The H atoms of the methyl groups were positioned with idealized geometry using a riding model with C—H = 0.96 Å. The other H atoms were located in difference map, and its positional parameters were refined freely [C—H = 0.87 (3)–1.05 (3) Å. All H atoms were refined with isotropic displacement parameters (U_{iso}(H) = 1.2 U_{eq}(CH) and 1.5U_{eq}(CH$_3$))

To improve the values of R1, wR2, and GOOF, the bad three reflections (1 1 0 2 0 0 1 1 1) were omitted from the refinement.
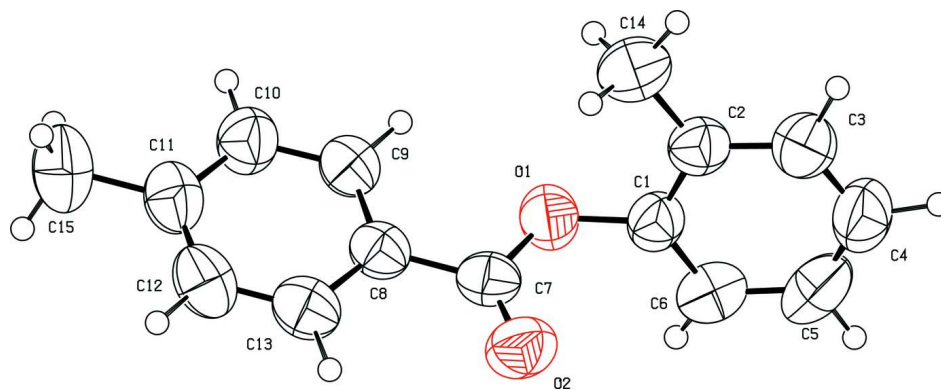
Figure 1

Molecular structure of the title compound, showing the atom labeling scheme. The displacement ellipsoids are drawn at the 50% probability level. The H atoms are represented as small spheres of arbitrary radii.
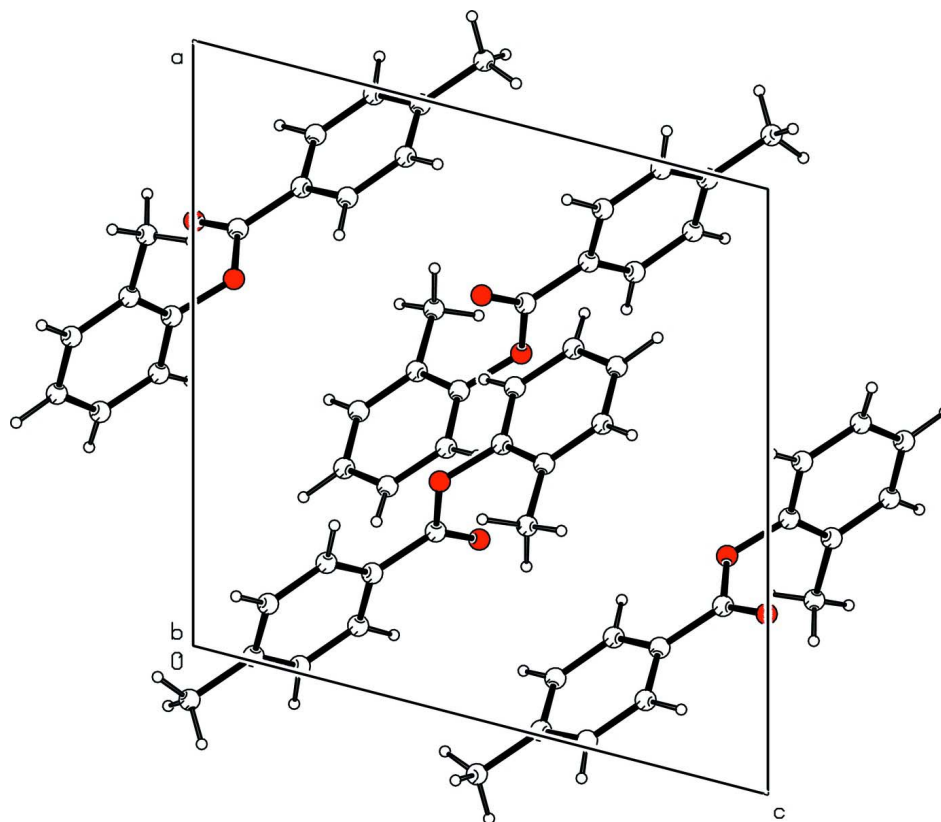
Figure 2

Molecular packing of the title compound.

2-Methylphenyl 4-methylbenzoate

Crystal data

$C_{15}H_{14}O_2$	$a = 11.690\ (2)$ Å
$M_r = 226.26$	$b = 9.670\ (1)$ Å
Monoclinic, $P2_1/c$	$c = 11.478\ (2)$ Å
Hall symbol: -P 2ybc	$\beta = 104.50\ (2)°$

$V = 1256.2$ (3) Å^3

$Z = 4$

$F(000) = 480$

$D_x = 1.196$ Mg m^{-3}

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1609 reflections

$\theta = 2.8–27.9°$

$\mu = 0.08$ mm^{-1}

$T = 299$ K

Prism, colourless

$0.50 \times 0.46 \times 0.20$ mm

Data collection

Oxford Diffraction Xcalibur
    diffractometer with a Sapphire CCD detector

Radiation source: fine-focus sealed tube

Graphite monochromator

Rotation method data acquisition using ω and φ
    scans

Absorption correction: multi-scan
    (*CrysAlis RED*; Oxford Diffraction, 2007)

$T_{min} = 0.968$, $T_{max} = 0.989$

7861 measured reflections

2529 independent reflections

1385 reflections with $I > 2\sigma(I)$

$R_{int} = 0.021$

$\theta_{max} = 26.4°$, $\theta_{min} = 2.8°$

$h = -11 \rightarrow 14$

$k = -12 \rightarrow 9$

$l = -13 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.053$

$wR(F^2) = 0.200$

$S = 1.04$

2529 reflections

181 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 atoms treated by a mixture of independent
    and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.092P)^2 + 0.342P]$
    where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.006$

$\Delta\rho_{max} = 0.21$ e Å^{-3}

$\Delta\rho_{min} = -0.15$ e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick,
    2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$

Extinction coefficient: 0.031 (6)

Special details

Experimental. empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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}
C1	0.5348 (2)	0.2164 (2)	0.4626 (2)	0.0639 (6)
C2	0.5493 (2)	0.1082 (2)	0.3892 (2)	0.0665 (6)
C3	0.4583 (3)	0.0849 (3)	0.2881 (2)	0.0818 (8)
H3	0.465 (2)	0.002 (3)	0.238 (3)	0.098*
C4	0.3581 (3)	0.1645 (4)	0.2630 (3)	0.0920 (9)
H4	0.293 (3)	0.134 (3)	0.192 (3)	0.110*

C5	0.3464 (3)	0.2706 (4)	0.3381 (3)	0.0929 (10)
H5	0.282 (3)	0.329 (3)	0.318 (3)	0.111*
C6	0.4355 (3)	0.2979 (3)	0.4402 (3)	0.0787 (8)
H6	0.436 (3)	0.363 (3)	0.493 (3)	0.094*
C7	0.7074 (2)	0.3305 (2)	0.5779 (2)	0.0642 (6)
C8	0.8038 (2)	0.3150 (2)	0.6887 (2)	0.0623 (6)
C9	0.8060 (2)	0.2066 (3)	0.7680 (2)	0.0713 (7)
H9	0.741 (2)	0.137 (3)	0.754 (2)	0.086*
C10	0.8988 (2)	0.1943 (3)	0.8698 (2)	0.0774 (7)
H10	0.901 (2)	0.116 (3)	0.926 (2)	0.093*
C11	0.9911 (2)	0.2878 (3)	0.8946 (2)	0.0786 (7)
C12	0.9879 (3)	0.3953 (3)	0.8146 (3)	0.0899 (9)
H12	1.052 (3)	0.462 (3)	0.823 (3)	0.108*
C13	0.8960 (2)	0.4098 (3)	0.7127 (3)	0.0802 (7)
H13	0.896 (2)	0.489 (3)	0.650 (2)	0.096*
C14	0.6588 (2)	0.0208 (3)	0.4190 (3)	0.0866 (8)
H14A	0.6673	−0.0210	0.4965	0.129*
H14B	0.7264	0.0777	0.4203	0.129*
H14C	0.6527	−0.0500	0.3592	0.129*
C15	1.0906 (3)	0.2722 (4)	1.0064 (3)	0.1079 (11)
H15A	1.1586	0.2344	0.9851	0.162*
H15B	1.0665	0.2111	1.0618	0.162*
H15C	1.1101	0.3610	1.0434	0.162*
O1	0.62322 (15)	0.23295 (16)	0.57090 (14)	0.0759 (5)
O2	0.70209 (16)	0.41780 (18)	0.50210 (17)	0.0858 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0637 (14)	0.0663 (13)	0.0593 (13)	−0.0023 (11)	0.0110 (11)	0.0084 (10)
C2	0.0723 (15)	0.0639 (13)	0.0640 (14)	0.0001 (11)	0.0183 (12)	0.0075 (11)
C3	0.097 (2)	0.0791 (17)	0.0654 (16)	−0.0007 (15)	0.0136 (14)	0.0045 (13)
C4	0.089 (2)	0.102 (2)	0.0721 (17)	−0.0112 (18)	−0.0030 (15)	0.0184 (17)
C5	0.0727 (19)	0.101 (2)	0.100 (2)	0.0197 (16)	0.0132 (17)	0.0367 (19)
C6	0.0850 (19)	0.0726 (15)	0.0808 (18)	0.0127 (14)	0.0252 (15)	0.0111 (13)
C7	0.0685 (15)	0.0544 (12)	0.0733 (15)	0.0050 (11)	0.0248 (12)	−0.0033 (11)
C8	0.0629 (13)	0.0598 (12)	0.0673 (14)	−0.0005 (10)	0.0220 (11)	−0.0064 (10)
C9	0.0678 (15)	0.0668 (14)	0.0770 (16)	−0.0082 (12)	0.0141 (13)	−0.0005 (12)
C10	0.0683 (16)	0.0829 (17)	0.0773 (17)	−0.0054 (13)	0.0115 (13)	0.0052 (13)
C11	0.0633 (15)	0.0930 (18)	0.0776 (17)	−0.0054 (13)	0.0140 (12)	−0.0117 (14)
C12	0.0740 (18)	0.0924 (19)	0.101 (2)	−0.0253 (15)	0.0165 (16)	−0.0105 (17)
C13	0.0813 (18)	0.0707 (15)	0.0899 (19)	−0.0129 (13)	0.0242 (15)	0.0009 (13)
C14	0.0866 (19)	0.0814 (17)	0.0954 (19)	0.0142 (14)	0.0294 (15)	0.0050 (14)
C15	0.0766 (19)	0.138 (3)	0.098 (2)	−0.0173 (18)	0.0013 (16)	−0.0083 (19)
O1	0.0790 (11)	0.0763 (11)	0.0667 (11)	−0.0141 (9)	0.0075 (8)	0.0060 (8)
O2	0.0901 (13)	0.0725 (11)	0.0936 (14)	0.0013 (9)	0.0205 (10)	0.0188 (9)

Geometric parameters (Å, º)

C1—C6	1.373 (3)	C8—C13	1.390 (3)
C1—C2	1.381 (3)	C9—C10	1.386 (4)
C1—O1	1.413 (3)	C9—H9	1.00 (3)
C2—C3	1.383 (4)	C10—C11	1.382 (4)
C2—C14	1.499 (3)	C10—H10	0.99 (3)
C3—C4	1.371 (4)	C11—C12	1.382 (4)
C3—H3	1.00 (3)	C11—C15	1.508 (4)
C4—C5	1.369 (4)	C12—C13	1.383 (4)
C4—H4	1.01 (3)	C12—H12	0.97 (3)
C5—C6	1.384 (4)	C13—H13	1.05 (3)
C5—H5	0.92 (3)	C14—H14A	0.9600
C6—H6	0.87 (3)	C14—H14B	0.9600
C7—O2	1.202 (3)	C14—H14C	0.9600
C7—O1	1.351 (3)	C15—H15A	0.9600
C7—C8	1.481 (3)	C15—H15B	0.9600
C8—C9	1.385 (3)	C15—H15C	0.9600
C6—C1—C2	123.3 (2)	C10—C9—H9	118.6 (15)
C6—C1—O1	119.9 (2)	C11—C10—C9	121.6 (3)
C2—C1—O1	116.6 (2)	C11—C10—H10	118.4 (16)
C1—C2—C3	116.7 (2)	C9—C10—H10	120.0 (16)
C1—C2—C14	121.1 (2)	C12—C11—C10	117.7 (3)
C3—C2—C14	122.2 (2)	C12—C11—C15	121.9 (3)
C4—C3—C2	121.5 (3)	C10—C11—C15	120.4 (3)
C4—C3—H3	121.1 (16)	C11—C12—C13	121.7 (3)
C2—C3—H3	117.2 (16)	C11—C12—H12	122.7 (18)
C5—C4—C3	120.2 (3)	C13—C12—H12	115.5 (18)
C5—C4—H4	123.4 (18)	C12—C13—C8	120.0 (3)
C3—C4—H4	116.1 (18)	C12—C13—H13	121.3 (15)
C4—C5—C6	120.2 (3)	C8—C13—H13	118.6 (15)
C4—C5—H5	120.5 (19)	C2—C14—H14A	109.5
C6—C5—H5	119 (2)	C2—C14—H14B	109.5
C1—C6—C5	118.1 (3)	H14A—C14—H14B	109.5
C1—C6—H6	115.4 (19)	C2—C14—H14C	109.5
C5—C6—H6	126.5 (19)	H14A—C14—H14C	109.5
O2—C7—O1	122.9 (2)	H14B—C14—H14C	109.5
O2—C7—C8	125.6 (2)	C11—C15—H15A	109.5
O1—C7—C8	111.49 (19)	C11—C15—H15B	109.5
C9—C8—C13	118.9 (2)	H15A—C15—H15B	109.5
C9—C8—C7	121.8 (2)	C11—C15—H15C	109.5
C13—C8—C7	119.3 (2)	H15A—C15—H15C	109.5
C8—C9—C10	120.1 (2)	H15B—C15—H15C	109.5
C8—C9—H9	121.4 (15)	C7—O1—C1	119.55 (17)
C6—C1—C2—C3	0.9 (4)	C13—C8—C9—C10	0.4 (4)
O1—C1—C2—C3	174.9 (2)	C7—C8—C9—C10	178.9 (2)

C6—C1—C2—C14	−179.0 (2)	C8—C9—C10—C11	−0.4 (4)
O1—C1—C2—C14	−4.9 (3)	C9—C10—C11—C12	0.3 (4)
C1—C2—C3—C4	−0.7 (4)	C9—C10—C11—C15	179.7 (3)
C14—C2—C3—C4	179.1 (2)	C10—C11—C12—C13	−0.1 (4)
C2—C3—C4—C5	0.4 (4)	C15—C11—C12—C13	−179.5 (3)
C3—C4—C5—C6	−0.3 (5)	C11—C12—C13—C8	0.1 (4)
C2—C1—C6—C5	−0.7 (4)	C9—C8—C13—C12	−0.2 (4)
O1—C1—C6—C5	−174.6 (2)	C7—C8—C13—C12	−178.8 (2)
C4—C5—C6—C1	0.4 (4)	O2—C7—O1—C1	10.7 (3)
O2—C7—C8—C9	−176.4 (2)	C8—C7—O1—C1	−169.31 (18)
O1—C7—C8—C9	3.7 (3)	C6—C1—O1—C7	−85.0 (3)
O2—C7—C8—C13	2.2 (4)	C2—C1—O1—C7	100.8 (2)
O1—C7—C8—C13	−177.7 (2)		