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4-Methylphenyl 4-methylbenzoate

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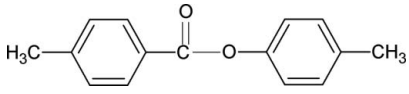
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.144; data-to-parameter ratio = 12.3.

The structure of the title compound, $C_{15}H_{14}O_2$, is similar to that of phenyl benzoate and 4-methylphenyl benzoate, with somewhat different bond parameters. The dihedral angle between the two aromatic rings is 63.57 (5)°.

Related literature

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



Experimental

Crystal data

$C_{15}H_{14}O_2$
M_r = 226.26
Monoclinic, $P2_1/n$
a = 6.113 (1) Å
b = 7.639 (1) Å
c = 26.510 (3) Å
β = 95.42 (1)°
V = 1232.4 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.64 mm^{-1}
T = 299 (2) K
0.53 × 0.33 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.782, T_{max} = 0.934
3680 measured reflections
2202 independent reflections
1858 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.144
S = 1.04
2202 reflections
179 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 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: BT2484).

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supplementary materials

Acta Cryst. (2007). E**63**, o3867 [**doi:10.1107/S1600536807040743**]

4-Methylphenyl 4-methylbenzoate

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

Comment

As part of a study of substituent effects on the structures of chemically and industrially significant compounds (Gowda *et al.*, 2007*a*, Gowda *et al.*, 2007*b*; Gowda, Kozisek *et al.*, 2007; Gowda, Foro, Nayak & Fuess, 2007), in the present work, the structure of 4-methylphenyl 4-methylbenzoate (4MeP4MeBA) has been determined. The structure of 4MeP4MeBA (Fig. 1) resembles that of phenyl benzoate (PBA) (Adams & Morsi, 1976) and 4-methylphenyl benzoate (4MePBA) (Gowda, Foro, Nayak & Fuess, 2007). The bond parameters in 4MeP4MeBA are similar to those in PBA, 4MePBA and other benzoates (Gowda *et al.*, 2007*a*, *b*). The molecules in the title compound are packed in to chains in the *ac* plane (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 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 their positions refined [C—H = 0.94 (2)–0.99 (2) Å]. All H atoms were refined with isotropic displacement parameters set to 1.2 times of the U_{eq} of the parent atom.

Figures

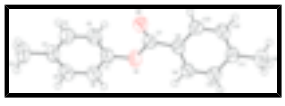

Fig. 1. Molecular structure of the title compound, showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius.

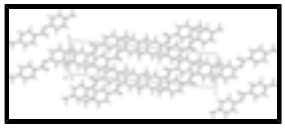

Fig. 2. Molecular packing of the title compound.

4-Methylphenyl 4-methylbenzoate

Crystal data

$C_{15}H_{14}O_2$	F_{000} = 480
M_r = 226.26	D_x = 1.219 Mg m^{-3}
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation

	λ = 1.54180 Å
Hall symbol: -P 2yn	Cell parameters from 25 reflections
a = 6.113 (1) Å	θ = 3.4–22.4º
b = 7.639 (1) Å	μ = 0.64 mm^{-1}
c = 26.510 (3) Å	T = 299 (2) K
β = 95.42 (1)º	Prism, colourless
V = 1232.4 (3) $Å^3$	0.53 × 0.33 × 0.10 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.018
Radiation source: fine-focus sealed tube	θ_{max} = 66.9º
Monochromator: graphite	θ_{min} = 3.4º
T = 299(2) K	h = 0→7
ω/2θ scans	k = −9→4
Absorption correction: ψ scan (North *et al.*, 1968)	l = −31→31
T_{min} = 0.782, T_{max} = 0.934	3 standard reflections
3680 measured reflections	every 120 min
2202 independent reflections	intensity decay: 1.0%
1858 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$w = 1/[\sigma^2(F_o^2) + (0.0792P)^2 + 0.2337P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.144	$(\Delta/\sigma)_{max} < 0.001$
S = 1.04	$\Delta\rho_{max}$ = 0.19 e $Å^{-3}$
2202 reflections	$\Delta\rho_{min}$ = −0.15 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: 0.0071 (10)
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	0.6081 (3)	0.8160 (2)	0.12177 (6)	0.0558 (4)
C2	0.7010 (3)	0.7320 (3)	0.08374 (7)	0.0662 (5)
H2	0.846 (3)	0.682 (3)	0.0905 (7)	0.079*
C3	0.5881 (3)	0.7227 (3)	0.03619 (7)	0.0666 (5)
H3	0.655 (3)	0.661 (3)	0.0092 (7)	0.080*
C4	0.3811 (3)	0.7961 (2)	0.02643 (6)	0.0588 (4)
C5	0.2931 (3)	0.8796 (2)	0.06581 (7)	0.0638 (5)
H5	0.145 (3)	0.932 (3)	0.0617 (7)	0.077*
C6	0.4036 (3)	0.8908 (2)	0.11347 (7)	0.0628 (4)
H6	0.345 (3)	0.951 (3)	0.1414 (8)	0.075*
C7	0.8771 (2)	0.93572 (19)	0.18165 (6)	0.0494 (4)
C8	0.9683 (2)	0.92623 (18)	0.23520 (5)	0.0472 (4)
C9	0.8641 (3)	0.8382 (2)	0.27175 (6)	0.0549 (4)
H9	0.724 (3)	0.782 (2)	0.2616 (6)	0.066*
C10	0.9581 (3)	0.8317 (2)	0.32113 (6)	0.0575 (4)
H10	0.888 (3)	0.768 (3)	0.3452 (7)	0.069*
C11	1.1604 (3)	0.90905 (19)	0.33506 (6)	0.0525 (4)
C12	1.2617 (3)	0.9984 (2)	0.29839 (6)	0.0593 (4)
H12	1.408 (3)	1.054 (2)	0.3062 (7)	0.071*
C13	1.1678 (3)	1.0089 (2)	0.24920 (6)	0.0564 (4)
H13	1.236 (3)	1.078 (2)	0.2247 (7)	0.068*
C14	0.2563 (4)	0.7841 (3)	−0.02516 (7)	0.0833 (6)
H14A	0.2982	0.6794	−0.0418	0.100*
H14B	0.2896	0.8842	−0.0450	0.100*
H14C	0.1014	0.7812	−0.0217	0.100*
C15	1.2671 (3)	0.8948 (3)	0.38833 (6)	0.0701 (5)
H15A	1.2080	0.7957	0.4047	0.084*
H15B	1.2387	0.9994	0.4067	0.084*
H15C	1.4228	0.8802	0.3876	0.084*
O1	0.7127 (2)	0.81850 (16)	0.17135 (4)	0.0690 (4)
O2	0.93656 (18)	1.03321 (16)	0.15041 (4)	0.0649 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0533 (8)	0.0618 (9)	0.0501 (8)	−0.0079 (7)	−0.0077 (6)	0.0050 (7)
C2	0.0534 (9)	0.0750 (11)	0.0677 (10)	0.0127 (8)	−0.0065 (8)	0.0021 (9)
C3	0.0653 (10)	0.0754 (11)	0.0579 (9)	0.0100 (9)	0.0001 (8)	−0.0063 (8)
C4	0.0597 (9)	0.0563 (9)	0.0573 (9)	−0.0027 (7)	−0.0110 (7)	0.0052 (7)

C5	0.0487 (8)	0.0677 (10)	0.0725 (10)	0.0060 (8)	−0.0079 (7)	0.0006 (8)
C6	0.0550 (9)	0.0720 (11)	0.0607 (9)	−0.0004 (8)	0.0027 (7)	−0.0072 (8)
C7	0.0431 (7)	0.0513 (8)	0.0531 (8)	0.0035 (6)	0.0015 (6)	0.0013 (6)
C8	0.0450 (7)	0.0463 (8)	0.0496 (8)	0.0024 (6)	0.0005 (6)	0.0001 (6)
C9	0.0474 (8)	0.0592 (9)	0.0568 (9)	−0.0078 (7)	−0.0013 (6)	0.0032 (7)
C10	0.0587 (9)	0.0621 (9)	0.0513 (8)	−0.0076 (7)	0.0030 (7)	0.0053 (7)
C11	0.0576 (8)	0.0479 (8)	0.0504 (8)	0.0023 (7)	−0.0029 (7)	−0.0049 (6)
C12	0.0526 (9)	0.0637 (10)	0.0599 (9)	−0.0120 (7)	−0.0038 (7)	−0.0052 (8)
C13	0.0535 (8)	0.0616 (9)	0.0537 (9)	−0.0110 (7)	0.0040 (7)	0.0018 (7)
C14	0.0895 (14)	0.0883 (14)	0.0659 (11)	−0.0005 (11)	−0.0254 (10)	0.0036 (10)
C15	0.0791 (12)	0.0728 (11)	0.0552 (9)	−0.0035 (9)	−0.0110 (8)	−0.0034 (8)
O1	0.0707 (7)	0.0798 (8)	0.0527 (7)	−0.0230 (6)	−0.0148 (5)	0.0114 (6)
O2	0.0622 (7)	0.0767 (8)	0.0550 (7)	−0.0098 (6)	0.0003 (5)	0.0121 (6)

Geometric parameters (Å, °)

C1—C2	1.364 (2)	C8—C13	1.392 (2)
C1—C6	1.374 (2)	C9—C10	1.380 (2)
C1—O1	1.4062 (18)	C9—H9	0.971 (18)
C2—C3	1.381 (2)	C10—C11	1.389 (2)
C2—H2	0.968 (19)	C10—H10	0.935 (18)
C3—C4	1.386 (2)	C11—C12	1.381 (2)
C3—H3	0.98 (2)	C11—C15	1.503 (2)
C4—C5	1.375 (2)	C12—C13	1.377 (2)
C4—C14	1.505 (2)	C12—H12	0.994 (19)
C5—C6	1.378 (2)	C13—H13	0.962 (18)
C5—H5	0.99 (2)	C14—H14A	0.9600
C6—H6	0.97 (2)	C14—H14B	0.9600
C7—O2	1.1957 (18)	C14—H14C	0.9600
C7—O1	1.3547 (18)	C15—H15A	0.9600
C7—C8	1.477 (2)	C15—H15B	0.9600
C8—C9	1.383 (2)	C15—H15C	0.9600
C2—C1—C6	120.92 (15)	C8—C9—H9	118.1 (10)
C2—C1—O1	120.89 (15)	C9—C10—C11	121.17 (15)
C6—C1—O1	118.06 (15)	C9—C10—H10	119.2 (11)
C1—C2—C3	119.48 (16)	C11—C10—H10	119.5 (11)
C1—C2—H2	119.2 (11)	C12—C11—C10	118.06 (14)
C3—C2—H2	121.3 (11)	C12—C11—C15	120.90 (15)
C2—C3—C4	121.23 (17)	C10—C11—C15	121.04 (15)
C2—C3—H3	119.0 (12)	C13—C12—C11	121.40 (15)
C4—C3—H3	119.8 (12)	C13—C12—H12	117.3 (11)
C5—C4—C3	117.49 (15)	C11—C12—H12	121.2 (11)
C5—C4—C14	121.14 (16)	C12—C13—C8	120.15 (15)
C3—C4—C14	121.37 (17)	C12—C13—H13	120.2 (11)
C4—C5—C6	122.13 (16)	C8—C13—H13	119.6 (11)
C4—C5—H5	121.6 (11)	C4—C14—H14A	109.5
C6—C5—H5	116.3 (11)	C4—C14—H14B	109.5
C1—C6—C5	118.75 (16)	H14A—C14—H14B	109.5
C1—C6—H6	118.3 (12)	C4—C14—H14C	109.5

C5—C6—H6	122.9 (12)	H14A—C14—H14C	109.5
O2—C7—O1	122.71 (14)	H14B—C14—H14C	109.5
O2—C7—C8	125.78 (14)	C11—C15—H15A	109.5
O1—C7—C8	111.52 (12)	C11—C15—H15B	109.5
C9—C8—C13	118.92 (14)	H15A—C15—H15B	109.5
C9—C8—C7	122.70 (13)	C11—C15—H15C	109.5
C13—C8—C7	118.38 (13)	H15A—C15—H15C	109.5
C10—C9—C8	120.25 (14)	H15B—C15—H15C	109.5
C10—C9—H9	121.6 (10)	C7—O1—C1	117.42 (12)
C6—C1—C2—C3	0.2 (3)	C13—C8—C9—C10	−0.5 (2)
O1—C1—C2—C3	176.04 (16)	C7—C8—C9—C10	179.20 (14)
C1—C2—C3—C4	−0.5 (3)	C8—C9—C10—C11	−1.6 (3)
C2—C3—C4—C5	0.4 (3)	C9—C10—C11—C12	2.3 (2)
C2—C3—C4—C14	−179.18 (18)	C9—C10—C11—C15	−177.20 (16)
C3—C4—C5—C6	−0.2 (3)	C10—C11—C12—C13	−1.0 (2)
C14—C4—C5—C6	179.43 (17)	C15—C11—C12—C13	178.51 (16)
C2—C1—C6—C5	0.0 (3)	C11—C12—C13—C8	−1.1 (3)
O1—C1—C6—C5	−175.92 (15)	C9—C8—C13—C12	1.8 (2)
C4—C5—C6—C1	0.0 (3)	C7—C8—C13—C12	−177.92 (14)
O2—C7—C8—C9	166.01 (15)	O2—C7—O1—C1	−1.0 (2)
O1—C7—C8—C9	−13.8 (2)	C8—C7—O1—C1	178.81 (13)
O2—C7—C8—C13	−14.3 (2)	C2—C1—O1—C7	80.2 (2)
O1—C7—C8—C13	165.92 (13)	C6—C1—O1—C7	−103.85 (18)

Fig. 1

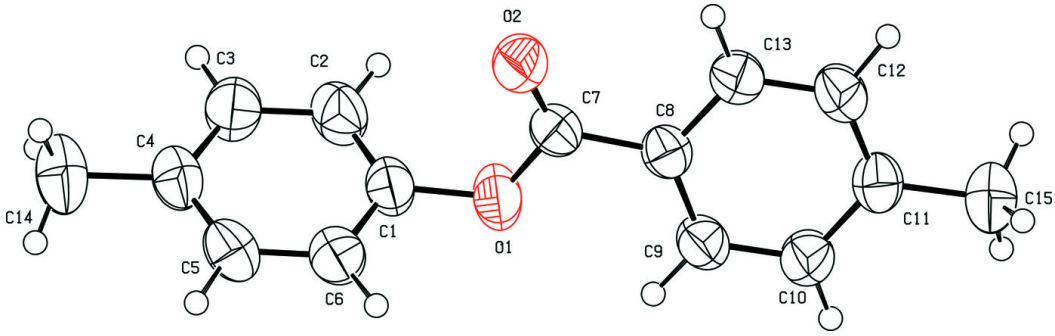

Fig. 2