

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Methyl 4-methylbenzoate

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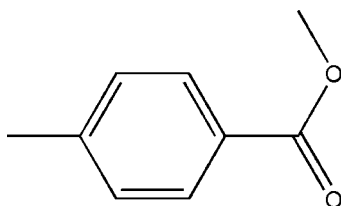
Received 29 March 2008; accepted 1 April 2008

Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.042; wR factor = 0.125; data-to-parameter ratio = 18.2.

The structure of the title compound, $\text{C}_9\text{H}_{10}\text{O}_2$, is related to that of 4-methylphenyl 4-methylbenzoate and ethylene di-4-methylbenzoate showing similar bond parameters. The molecule is planar, the dihedral angle between the aromatic ring and the $-\text{COOMe}$ group being 0.95 (6)°. The crystal structure exhibits intermolecular $\text{C}-\text{H}\cdots\text{O}$ contacts that link molecules into infinite chains extended in the $[001]$ direction.

Related literature

For related literature, see: Deguire & Brisse (1988); Gowda *et al.* (2007); Gray & Whalley (1971); Harris & Mantle (2001); Saeed & Rama (1994); Simpson (1978).



Experimental

Crystal data

$\text{C}_9\text{H}_{10}\text{O}_2$
 $M_r = 150.17$
 Monoclinic, $P2_1/c$

$a = 5.9134$ (11) Å
 $b = 7.6048$ (14) Å
 $c = 17.484$ (3) Å

$\beta = 97.783$ (4)°
 $V = 779.0$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.09$ mm⁻¹
 $T = 120$ (2) K
 $0.45 \times 0.43 \times 0.39$ mm

Data collection

Bruker SMART APEX diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2004)
 $T_{\min} = 0.961$, $T_{\max} = 0.967$

6617 measured reflections
 1855 independent reflections
 1482 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.124$
 $S = 1.06$
 1855 reflections

102 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.31$ e Å⁻³
 $\Delta\rho_{\min} = -0.20$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C9}-\text{H9B}\cdots\text{O2}^i$	0.98	2.51	3.4930 (16)	177

Symmetry code: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

AS gratefully acknowledges a research grant from Quaid-I-Azam University, Islamabad.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2231).

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supplementary materials

Acta Cryst. (2008). E64, o821 [doi:10.1107/S1600536808008738]

Methyl 4-methylbenzoate

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Comment

The title ester is an important intermediate in the synthesis of a variety of natural products. These include the sclerotiorin group of fungal metabolites (Gray & Whalley, 1971), isochromans related to sclerotiorin pigments (Saeed & Rama, 1994) and isocoumarins like the 7-methylmellein (Harris & Mantle, 2001) and stellatin (Simpson, 1978).

Experimental

The title ester was prepared from commercial *p*-toluic acid according to standard procedure.

Refinement

Hydrogen atoms were located in difference syntheses, refined at idealized positions riding on the carbon or nitrogen atoms ($C-H = 0.88-0.99 \text{ \AA}$) with isotropic displacement parameters $U_{iso}(H) = 1.2U(C_{eq})$.

Figures

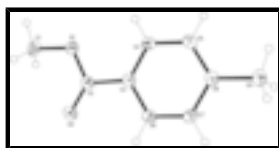


Fig. 1. Molecular structure of title compound. Displacement ellipsoids are drawn at the 50% probability level.



Fig. 2. Crystal packing viewed along [100] with intermolecular hydrogen bonding pattern indicated as dashed lines. H-atoms not involved in hydrogen bonding are omitted.

Methyl 4-methylbenzoate

Crystal data

$C_9H_{10}O_2$

$M_r = 150.17$

Monoclinic, $P2_1/c$

Hall symbol: $-P 2_1/c$

$a = 5.9134 (11) \text{ \AA}$

$b = 7.6048 (14) \text{ \AA}$

$c = 17.484 (3) \text{ \AA}$

$\beta = 97.783 (4)^\circ$

$V = 779.0 (2) \text{ \AA}^3$

$F_{000} = 320$

$D_x = 1.280 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 806 reflections

$\theta = 2.4-27.8^\circ$

$\mu = 0.09 \text{ mm}^{-1}$

$T = 120 (2) \text{ K}$

Block, colourless

$0.45 \times 0.43 \times 0.39 \text{ mm}$

supplementary materials

Z = 4

Data collection

Bruker SMART APEX diffractometer	1855 independent reflections
Radiation source: sealed tube	1482 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.039$
$T = 120(2)$ K	$\theta_{\text{max}} = 27.9^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.4^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$h = -7 \rightarrow 7$
$T_{\text{min}} = 0.961$, $T_{\text{max}} = 0.967$	$k = -10 \rightarrow 9$
6617 measured reflections	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.124$	$w = 1/[\sigma^2(F_o^2) + (0.0752P)^2 + 0.0208P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
1855 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
102 parameters	$\Delta\rho_{\text{max}} = 0.31 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.20 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.39091 (14)	0.28701 (11)	0.44793 (5)	0.0280 (2)
O2	0.68910 (15)	0.15425 (13)	0.51751 (5)	0.0325 (3)
C1	0.2956 (2)	0.31740 (17)	0.51874 (7)	0.0320 (3)
H1A	0.2793	0.2050	0.5448	0.048*
H1B	0.1456	0.3732	0.5068	0.048*

H1C	0.3974	0.3946	0.5526	0.048*
C2	0.59091 (19)	0.20144 (15)	0.45593 (6)	0.0234 (3)
C3	0.67753 (18)	0.17434 (15)	0.38071 (6)	0.0223 (3)
C4	0.55841 (19)	0.23124 (15)	0.31083 (7)	0.0247 (3)
H4A	0.4154	0.2888	0.3098	0.030*
C5	0.6496 (2)	0.20350 (15)	0.24261 (7)	0.0262 (3)
H5A	0.5675	0.2426	0.1952	0.031*
C6	0.8588 (2)	0.11953 (15)	0.24239 (7)	0.0244 (3)
C7	0.97615 (19)	0.06389 (15)	0.31291 (7)	0.0253 (3)
H7A	1.1195	0.0068	0.3140	0.030*
C8	0.88716 (19)	0.09050 (15)	0.38126 (7)	0.0242 (3)
H8A	0.9693	0.0515	0.4287	0.029*
C9	0.9593 (2)	0.08897 (17)	0.16858 (7)	0.0312 (3)
H9A	1.1213	0.1213	0.1764	0.047*
H9B	0.8782	0.1613	0.1273	0.047*
H9C	0.9438	-0.0355	0.1542	0.047*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0268 (5)	0.0322 (5)	0.0260 (4)	0.0042 (3)	0.0071 (3)	0.0018 (3)
O2	0.0343 (5)	0.0389 (5)	0.0234 (5)	0.0042 (4)	0.0004 (4)	0.0016 (3)
C1	0.0340 (7)	0.0342 (7)	0.0299 (7)	0.0024 (5)	0.0121 (5)	-0.0009 (5)
C2	0.0249 (6)	0.0201 (6)	0.0248 (6)	-0.0033 (4)	0.0022 (5)	0.0003 (4)
C3	0.0236 (6)	0.0203 (6)	0.0232 (6)	-0.0031 (4)	0.0031 (4)	0.0006 (4)
C4	0.0214 (5)	0.0252 (6)	0.0271 (6)	0.0008 (4)	0.0022 (4)	0.0024 (4)
C5	0.0271 (6)	0.0281 (6)	0.0222 (6)	-0.0019 (5)	-0.0006 (5)	0.0029 (4)
C6	0.0275 (6)	0.0210 (6)	0.0251 (6)	-0.0058 (4)	0.0049 (4)	-0.0010 (4)
C7	0.0231 (6)	0.0215 (6)	0.0316 (6)	0.0008 (4)	0.0042 (5)	0.0002 (4)
C8	0.0245 (6)	0.0221 (6)	0.0251 (6)	-0.0017 (4)	0.0000 (4)	0.0032 (4)
C9	0.0355 (7)	0.0320 (7)	0.0271 (6)	-0.0005 (5)	0.0079 (5)	-0.0018 (5)

Geometric parameters (\AA , $^\circ$)

O1—C2	1.3405 (14)	C5—C6	1.3927 (17)
O1—C1	1.4468 (14)	C5—H5A	0.9500
O2—C2	1.2065 (14)	C6—C7	1.3962 (17)
C1—H1A	0.9800	C6—C9	1.5101 (16)
C1—H1B	0.9800	C7—C8	1.3843 (16)
C1—H1C	0.9800	C7—H7A	0.9500
C2—C3	1.4890 (16)	C8—H8A	0.9500
C3—C8	1.3929 (16)	C9—H9A	0.9800
C3—C4	1.3940 (16)	C9—H9B	0.9800
C4—C5	1.3899 (16)	C9—H9C	0.9800
C4—H4A	0.9500		
C2—O1—C1	115.38 (9)	C4—C5—H5A	119.3
O1—C1—H1A	109.5	C6—C5—H5A	119.3
O1—C1—H1B	109.5	C5—C6—C7	118.16 (10)

supplementary materials

H1A—C1—H1B	109.5	C5—C6—C9	121.71 (11)
O1—C1—H1C	109.5	C7—C6—C9	120.13 (11)
H1A—C1—H1C	109.5	C8—C7—C6	121.10 (10)
H1B—C1—H1C	109.5	C8—C7—H7A	119.5
O2—C2—O1	123.28 (10)	C6—C7—H7A	119.5
O2—C2—C3	124.43 (11)	C7—C8—C3	120.20 (10)
O1—C2—C3	112.28 (9)	C7—C8—H8A	119.9
C8—C3—C4	119.46 (10)	C3—C8—H8A	119.9
C8—C3—C2	118.00 (10)	C6—C9—H9A	109.5
C4—C3—C2	122.54 (10)	C6—C9—H9B	109.5
C5—C4—C3	119.76 (11)	H9A—C9—H9B	109.5
C5—C4—H4A	120.1	C6—C9—H9C	109.5
C3—C4—H4A	120.1	H9A—C9—H9C	109.5
C4—C5—C6	121.33 (10)	H9B—C9—H9C	109.5
C1—O1—C2—O2	-1.07 (16)	C3—C4—C5—C6	0.00 (17)
C1—O1—C2—C3	179.72 (9)	C4—C5—C6—C7	-0.20 (17)
O2—C2—C3—C8	-0.70 (18)	C4—C5—C6—C9	-179.94 (10)
O1—C2—C3—C8	178.50 (10)	C5—C6—C7—C8	0.28 (17)
O2—C2—C3—C4	-179.94 (11)	C9—C6—C7—C8	-179.98 (10)
O1—C2—C3—C4	-0.74 (16)	C6—C7—C8—C3	-0.16 (17)
C8—C3—C4—C5	0.12 (17)	C4—C3—C8—C7	-0.05 (17)
C2—C3—C4—C5	179.36 (10)	C2—C3—C8—C7	-179.32 (10)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9—H9B \cdots O2 ⁱ	0.98	2.51	3.4930 (16)	177

Symmetry codes: (i) $x, -y+1/2, z-1/2$.

Fig. 1

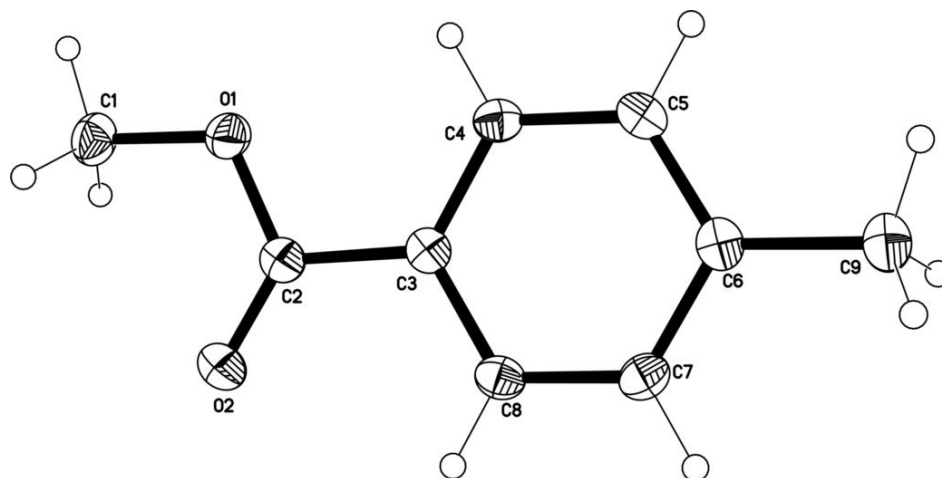


Fig. 2

