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Methyl 4-bromobenzoate

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.006 Å
R factor = 0.041
wR factor = 0.093
Data-to-parameter ratio = 13.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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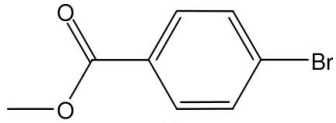
Molecules of the title compound, $C_8H_7BrO_2$, are almost planar. The compound is isostructural with methyl 4-iodobenzoate but not with methyl 4-chlorobenzoate. The crystal packing is characterized by a short Br···O interaction of 3.047 (3) Å.

Comment

The crystal structures of methyl 4-iodobenzoate (Brock, 1987) and methyl 4-chlorobenzoate (Roy *et al.*, 1993) have already been determined, but the structure of methyl 4-bromobenzoate, (I), was missing until now.



(I)

A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27 plus one update; *MOGUL* Version 1.1; Allen, 2002). The molecule is essentially planar (r.m.s. deviation for all non-H atoms = 0.092 Å). It is interesting that (I) is isostructural with the iodo compound (Brock, 1987), but not with the chloro compound (Roy *et al.*, 1993). The crystal structure is stabilized by a short Br···O contact [Br1···O1^{i} = 3.047 (3) Å and Br1···O1^{i}—C7^{i} = 146.7 (3)°; symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$]. The shortest Br···Br contact is 4.759 (1) Å; symmetry code to generate the second Br atom: $-x+\frac{1}{2}, y-\frac{1}{2}, z$]. Similar short contacts were noted in the iodo compound where the shortest I···I contact is 4.863 (1) Å and the shortest distance between I and the carbonyl O is 3.203 (4) Å. The molecules crystallize in chains (Fig. 2). The angle between two molecules in a chain is 38.04 (8)°.

Experimental

The title compound was purchased from Lancaster Synthesis, England, and recrystallized from an ethanol solution.

Crystal data

$C_8H_7BrO_2$
M_r = 215.05
Orthorhombic, *Pbca*
a = 13.8485 (18) Å
b = 5.8921 (8) Å
c = 19.613 (2) Å
V = 1600.4 (3) Å^3
Z = 8
D_x = 1.785 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6406 reflections
θ = 2.4–24.9°
μ = 5.08 mm^{-1}
T = 173 (2) K
Needle, colourless
0.31 × 0.10 × 0.06 mm

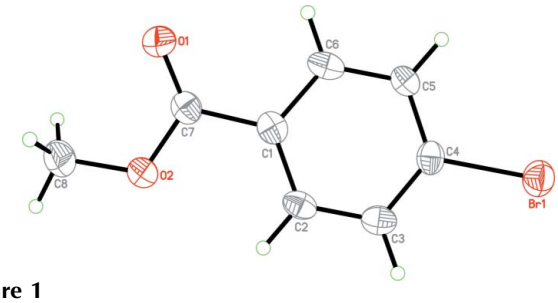


Figure 1
Perspective view of the title compound, showing the atom numbering and displacement ellipsoids drawn at the 50% probability level.

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.302, T_{max} = 0.750
10202 measured reflections
1375 independent reflections
998 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 25.0°
$h = -15 \rightarrow 15$
$k = -6 \rightarrow 6$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.093
S = 0.94
1375 reflections
101 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—C4	1.900 (4)	O2—C7	1.345 (5)
O1—C7	1.201 (6)		
C7—O2—C8	115.3 (4)	O1—C7—O2	123.7 (4)
C5—C4—Br1	119.1 (3)	O1—C7—C1	125.0 (4)
C3—C4—Br1	119.3 (3)	O2—C7—C1	111.3 (4)

H atoms were located in a difference map but positioned geometrically and refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C) or 1.5 U_{eq}(methyl C)] using a riding model, with C—H = 0.95 and 0.98 Å for aromatic and methyl H atoms, respectively. The methyl group was allowed to rotate but not to tip.

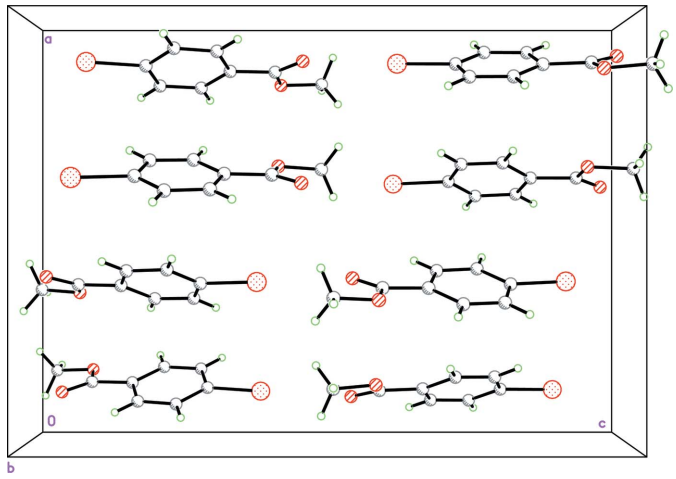


Figure 2
Packing of the title compound, viewed along the *b* axis.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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