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Methyl 4-(bromomethyl)benzoate

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.005 Å
R factor = 0.048
wR factor = 0.123
Data-to-parameter ratio = 19.5

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

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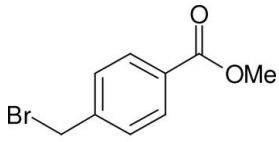
The ester group of the title compound, $C_9H_9BrO_2$, is only slightly twisted out of the plane of the central aromatic ring. Geometric parameters are in the usual ranges.

Comment

The title compound, (I), is a lachrymator and a drug intermediate. Methyl 4-(bromomethyl)benzoate is widely employed in synthetic organic chemistry and has wide applications (Liu *et al.*, 2001; Tang *et al.*, 2006). Recently, the title compound was used to synthesize methyl 4-[(2-butyl-4-chloro-5-formyl-1*H*-imidazol-1-yl)methyl]benzoate (Yang *et al.*, 2004). In addition, methyl 4-(bromomethyl)benzoate has been used in the synthesis of 1-(carboxybenzy1)imidazole-5-acrylic acids, which are potent and selective angiotensin II receptor antagonists (Weinstock *et al.*, 1991).



(I)

A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.28, November 2006; *Mogul* Version 1.1; Allen, 2002, Bruno *et al.*, 2004). The ester group is twisted by only 9.88 (19)° out of the plane of the central aromatic ring. There are no short C—H···*X* contacts, but one π–π stacking interaction can be observed in the crystal packing (Fig. 2). Carboxylate atom C7 is located above the centre of the aromatic ring of a neighboring parallel molecule (at $x-1$, y, z) at a distance of 3.585 Å.

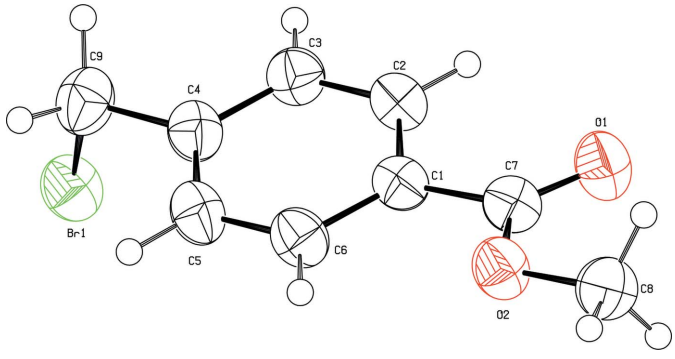


Figure 1
The molecular structure of the title compound with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

Experimental

N-Bromosuccinimide (23.9 g, 0.133 mol) and benzoyl peroxide (0.41 g, 0.0017 mol) were added to methyl 4-methylbenzoate (20 g, 0.133 mol) in 100 ml carbon tetrachloride and heated to reflux while irradiating with light (IR lamp). The reaction mixture was filtered and the filtrate was concentrated after washing with $NaHCO_3$ solution and dried over anhydrous Na_2SO_4. The resulting title compound was crystallized by slow evaporation of a solution in acetone (yield 75%; m.p. 325–327 K). Analysis found/calculated (%) for $C_9H_9BrO_2$: C 47.01/47.19, H 3.88/3.96.

Crystal data

$C_9H_9BrO_2$
M_r = 229.07
Orthorhombic, $P2_12_12_1$
a = 4.4481 (3) Å
b = 6.1860 (3) Å
c = 33.048 (2) Å
V = 909.35 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.47 mm^{-1}
T = 173 (2) K
0.25 × 0.13 × 0.12 mm

Data collection

Stoe IPDS-II two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.401, T_{max} = 0.616 (expected range = 0.380–0.584)
13106 measured reflections
2164 independent reflections
2052 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.123
S = 1.05
2164 reflections
111 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}
Absolute structure: Flack (1983), 837 Friedel pairs
Flack parameter: 0.002 (18)

H atoms were found in a difference map, but were refined using a riding model, with C—H = 0.95–0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(methyl C). The methyl groups were allowed to rotate but not to tip.

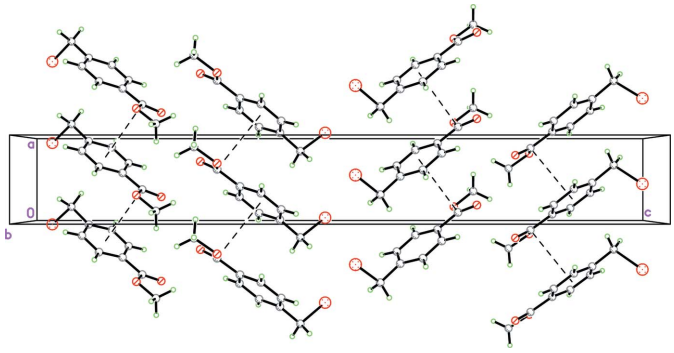


Figure 2
Packing diagram of the title compound. π–π Stacking interactions shown as dashed lines.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; 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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