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(*E*)-Methyl 3-[3-(bromomethyl)phenyl]acrylate

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Key indicators

Single-crystal X-ray study
T = 300 K
Mean σ(C–C) = 0.005 Å
R factor = 0.039
wR factor = 0.108
Data-to-parameter ratio = 16.3

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

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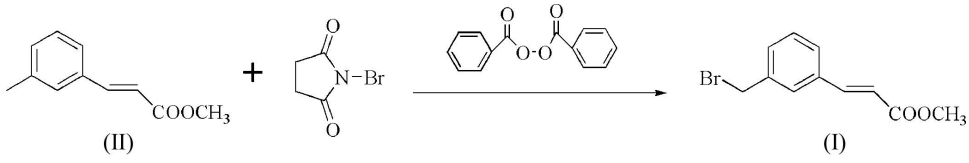
In the title molecule, $C_{11}H_{11}BrO_2$, all bond lengths and angles show normal values. Weak intermolecular C—H···O hydrogen bonds link the molecules into centrosymmetric dimers and C—H···π interactions contribute to the stability of the crystal packing.

Comment

Acrylate and its derivatives are used in the sythesis of acrylic resins, which have important commercial applications in the paint industry (Seda & Vural, 2005). Here we report the crystal structure of the title compound, (I) (Fig. 1).



The bond lengths and angles in (I) show normal values (Allen *et al.*, 1987). The mean plane through O1/O2/C9–C11 and the benzene ring make a dihedral angle of 9.20 (2)°.

Weak intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into centrosymmetric dimers (Fig. 2) and weak C—H···π interactions (Table 1) contribute to the stability of the crystal packing (Janiak, 2000).

Experimental

(*E*)-Methyl 3-*m*-tolylacrylate, (II), was prepared according to a literature procedure (List *et al.*, 2006) in 85% yield. To a solution of compound (II) (5 mmol) in carbon tetrachloride (20 ml) was added *N*-bromosuccinimide (6 mmol) and dibenzoyl peroxide (1.2 mmol).

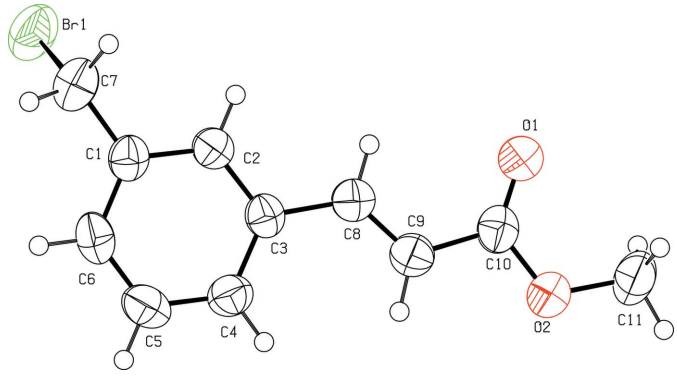


Figure 1
The molecular structure of (I), showing the labelling scheme and 50% probability displacement ellipsoids.

The mixture was stirred at 350K for 8 h, then washed with water and 4% NaOH solution in water. The solvent was removed under reduced pressure and the residue was purified by chromatography (silica gel with 3% ethyl acetate in petroleum ether). Recrystallization from hexane and dichloromethane (5:1) over a period of one week gave colourless crystals of (I).

Crystal data

$C_{11}H_{11}BrO_2$
M_r = 255.11
Triclinic, $P\overline{1}$
a = 6.1578 (5) Å
b = 7.8390 (7) Å
c = 12.0604 (10) Å
α = 77.580 (1)°
β = 88.816 (1)°
γ = 71.594 (1)°
V = 538.76 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.79 mm^{-1}
T = 300 (2) K
0.30 × 0.30 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
4156 measured reflections
2097 independent reflections
1698 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.108
S = 1.07
2097 reflections
129 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.93	2.59	3.369 (4)	141
C11—H11A···Cg^{ii}	0.96	2.82	3.6048	140

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x+1, -y+2, -z$. Cg is the centroid of the benzene ring.

All H atoms were positioned geometrically (C—H 0.93–0.97 Å) and refined using a riding model, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

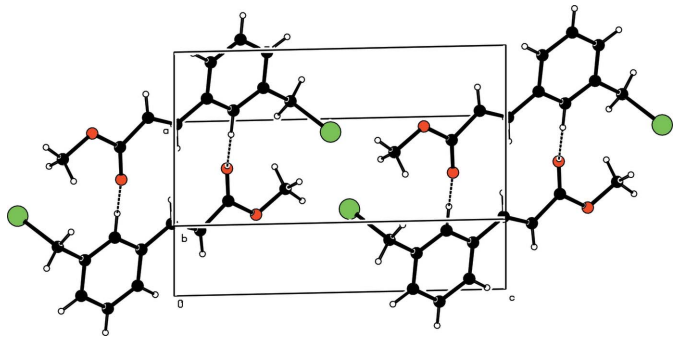


Figure 2
A portion of the crystal packing, showing the C—H···O hydrogen-bonded (dashed lines) centrosymmetric dimers.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: Bruker *SHELXTL* (Bruker, 1997); software used to prepare material for publication: Bruker *SHELXTL*.

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