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# 3-(4-Bromophenyl)-2-methylacrylic acid

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**Key indicators**

Single-crystal X-ray study
$T$ = 100 K
Mean $\sigma$(C–C) = 0.004 Å
$R$ factor = 0.033
$wR$ factor = 0.087
Data-to-parameter ratio = 13.8

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



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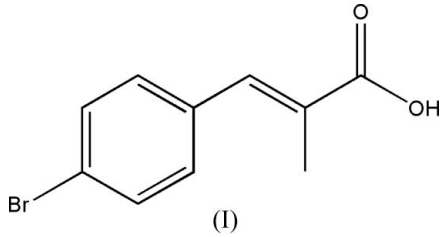
The title compound, $C_{10}H_9BrO_2$, displays an *E* configuration about the C=C double bond. In the crystal structure, symmetry-related molecules are linked by O—H···O hydrogen bonds, forming centrosymmetric carboxylic acid dimers.

## Comment

Cinnamic acid and its derivatives have been reported to possess a variety of pharmacological properties, including hepatoprotective (Perez-Alvarez *et al.*, 2001), antimalarial (Wiesner *et al.*, 2001), antioxidant (Natella *et al.*, 1999) and antihyperglycemic activities (Liu *et al.*, 1999). They constitute a large family of organic acids that have antibacterial, antifungal and antiparasitic activities, as well as antitumour and chemopreventive properties (Liu *et al.*, 1995). The molecular structure of compound (I) is shown in Fig. 1, and selected bond distances and angles are given in Table 1. The C7—C8 bond length of 1.349 (3) Å shows it to have double bond character, and the configuration about this bond is *E*. The bond lengths within the benzene ring range from 1.389 (4) to 1.403 (3) Å, typical of aromatic character (Allen *et al.*, 1987). Intermolecular hydrogen bonding between carboxyl groups in the crystal structure of (I) results in the formation of dimers. These dimers are further linked by intermolecular C—H···O bonds, forming a chain-like structure. (Table 2 and Fig. 2).




(I)

## Experimental

Compound (I) was synthesized according to a reported method (Gensler & Berman, 1958). A mixture of 4-bromobenzaldehyde (1.85 g, 10 mmol), methylmalonic acid (2.36 g, 20 mmol) and piperidine (1.98 ml, 20 mmol) in pyridine solvent (12.5 ml) was heated on a steam bath for 24 h. The reaction mixture was cooled and added to a mixture of 25 ml of concentrated HCl and 50 g of ice. The precipitate formed in the acidified mixture was filtered off and washed with ice-cold water. The product was recrystallized from ethanol. The yield was 90%.

*Crystal data*

$C_{10}H_9BrO_2$
$M_r$ = 241.08
Triclinic, $P\overline{1}$
$a$ = 7.3202 (11) Å
$b$ = 8.1460 (13) Å
$c$ = 9.0526 (14) Å
$\alpha$ = 114.431 (2)°
$\beta$ = 107.444 (2)°
$\gamma$ = 92.065 (2)°
$V$ = 460.85 (12) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 4.42 mm$^{-1}$
$T$ = 100 (1) K
0.44 × 0.17 × 0.14 mm

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
$T_{min}$ = 0.243, $T_{max}$ = 0.539
3745 measured reflections
2129 independent reflections
1932 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.087
$S$ = 1.03
2129 reflections
154 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 1.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.78 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Br—C3 | 1.897 (3) | O2—C9 | 1.232 (3) |
| O1—C9 | 1.321 (3) | C7—C8 | 1.349 (3) |
| | | | |
| Br—C3—C4 | 118.1 (2) | O2—C9—C8 | 121.4 (2) |
| Br—C3—C2 | 120.49 (19) | O1—C9—O2 | 122.4 (3) |
| O1—C9—C8 | 116.2 (2) | | |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H11···O2$^{i}$ | 0.81 (5) | 1.83 (5) | 2.646 (3) | 177 (7) |
| C2—H2···O2$^{ii}$ | 1.03 (3) | 2.46 (3) | 3.447 (3) | 160 (3) |
| C7—H7···O1 | 0.99 (3) | 2.36 (4) | 2.729 (4) | 101 (2) |

Symmetry codes: (i) $-x+3, -y, -z+1$; (ii) $x-1, y, z-1$.

All H atoms were located in a difference Fourier map and were refined with isotropic displacement parameters. The refined C—H distances are in the range 0.92 (4)–1.04 (4) Å. The highest residual density peak is located 1.0 Å from the Br atom.

Data collection: *SMART* (Bruker, 2006); cell refinement: *SAINT-Plus* (Bruker, 2006); data reduction: *SAINT-Plus*; program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLUTO* (Meetsma, 2007) and *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

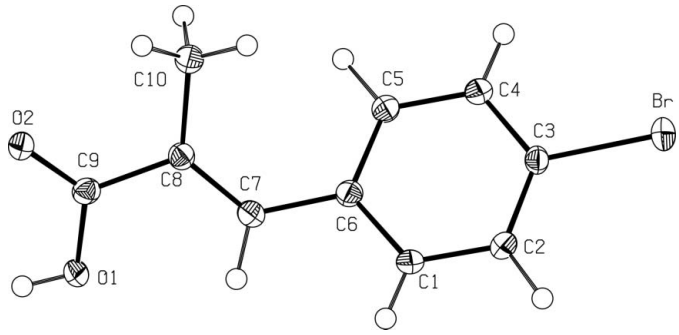



**Figure 1**
The molecular structure of the title compound. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. H atoms are drawn with an arbitrary radius.

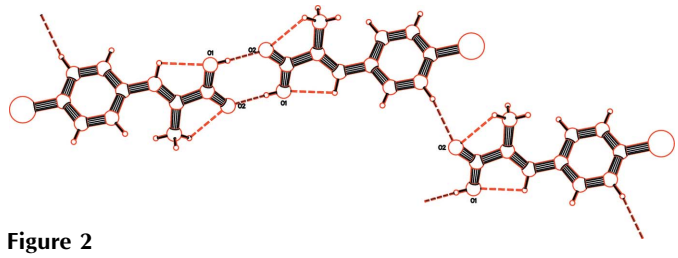


**Figure 2**
Perspective drawing of the dimer formed by O—H···O hydrogen bonds and the connection by C—H···O interactions to give a chain.

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