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(*E*)-Methyl 3-{3-[(4-bromophenoxy)-methyl]phenyl}acrylate

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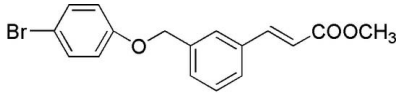
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.005 Å; R factor = 0.054; wR factor = 0.162; data-to-parameter ratio = 16.5.

In the molecule of the title compound, $C_{17}H_{15}BrO_3$, the rings make a dihedral angle of 75.54 (17)°. In the crystal structure, intermolecular C—H···O hydrogen bonds link the molecules into centrosymmetric dimers, and the π-stacked dimers interact with neighbouring dimers via C—H···π stacking interactions.

Related literature

For general background, see: de Fraine *et al.* (1991); Zhang & Ji (1992); Janiak (2000). For related literature, see: Ren *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{17}H_{15}BrO_3$
M_r = 347.20
Orthorhombic, *Pbca*
a = 15.5226 (9) Å
b = 5.9390 (3) Å
c = 34.775 (2) Å
V = 3205.9 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.57 mm^{-1}
T = 292 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001*a*)
T_{min} = 0.627, T_{max} = 0.783
30716 measured reflections
3147 independent reflections
1604 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.162
S = 1.02
3147 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

*Cg*2 is the centroid of the ring C1–C6.

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O2^{i}	0.93	2.45	3.370 (6)	172
C12—H12···*Cg*2^{ii}	0.93	2.99	3.677 (3)	132

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y-\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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: *SHELXTL* (Sheldrick, 2001*b*).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2392).

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supporting information

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(*E*)-Methyl 3-{3-[(4-bromophenoxy)methyl]phenyl}acrylate

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S1. Comment

Phenyl acrylate and its derivatives are important compounds because of their agrochemical and medical applications (de Fraine *et al.*, 1991; Zhang & Ji, 1992). We report herein the crystal structure of the title compound, (I).

In the molecule of (I), (Fig. 1) the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings A (C1—C6) and B (C8—C13) are, of course, planar, and they are oriented at a dihedral angle of A/B = 75.54 (17)°.

In the crystal structure, intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into centrosymmetric dimers (Fig. 2) and the π-stacked dimers interact with neighbouring dimers *via* C–H/π stacking interactions (Table 1) (Janiak, 2000), in which both of them seem to be effective in the stabilization of the structure.

S2. Experimental

(*E*)-methyl 3-(3-(bromomethyl)phenyl)acrylate, (II), was firstly synthesized, (yield; 52.8%), according to a literature method (Ren *et al.*, 2007). For the preparation of the title compound, (I), 4-bromophenol (2.0 mmol) and potassium carbonate (1.2 mmol) was added to a solution of compound (II) (2.0 mmol) in acetone (30 ml). The mixture was stirred at 329 K for 5 h, the solvent was removed under reduced pressure, and the residue was purified by chromatography (silica gel with 5% ethyl acetate in petroleum ether). Colorless crystals of (I) suitable for X-ray analysis were grown from methanol.

S3. Refinement

H atoms were positioned geometrically, with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

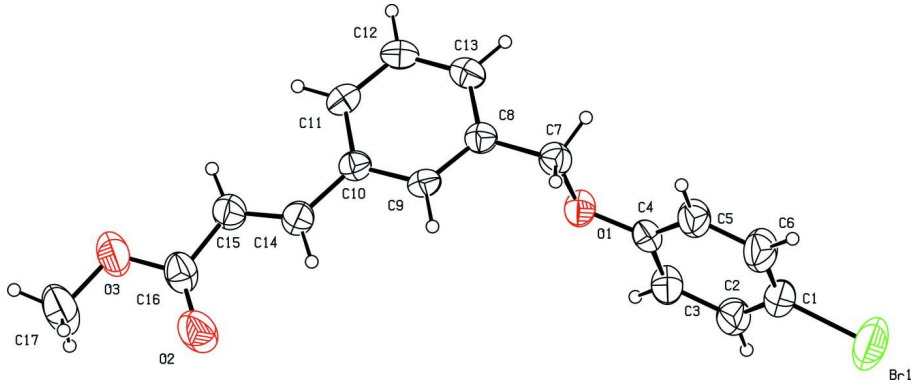


Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

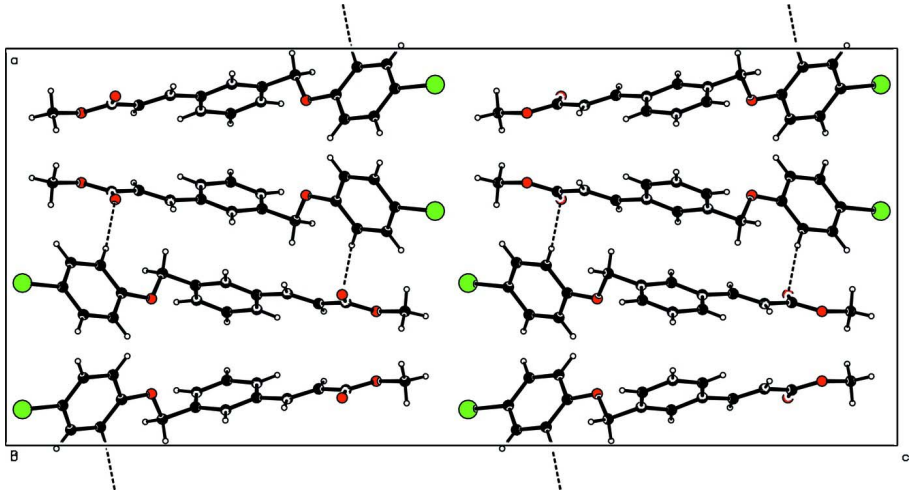
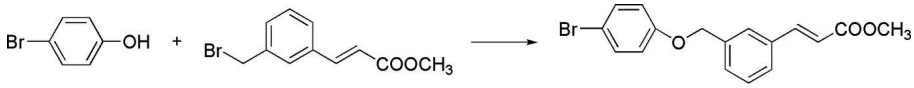


Figure 2

A packing diagram of (I). Hydrogen bonds are shown as dashed lines.



II I

Figure 3

The formation of the title compound.

(*E*)-Methyl 3-{3-[(4-bromophenoxy)methyl]phenyl}acrylate

Crystal data

$C_{17}H_{15}BrO_3$
$M_r = 347.20$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 15.5226\ (9)$ Å
$b = 5.9390\ (3)$ Å
$c = 34.775\ (2)$ Å
$V = 3205.9\ (3)$ Å^3
$Z = 8$
$F(000) = 1408$
$D_x = 1.439$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3230 reflections
$\theta = 2.3$–$18.7°$
$\mu = 2.57$ mm^{-1}
$T = 292$ K
Block, colorless
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001a)
$T_{min} = 0.627$, $T_{max} = 0.783$
30716 measured reflections
3147 independent reflections
1604 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.8°$
$h = -19 \rightarrow 19$
$k = -7 \rightarrow 7$
$l = -39 \rightarrow 42$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.162$
$S = 1.02$
3147 reflections
191 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0796P)^2 + 0.4215P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.40930 (5)	0.23555 (10)	0.518514 (16)	0.1544 (4)
O1	0.36979 (14)	0.7793 (4)	0.66326 (7)	0.0701 (7)
O2	0.3798 (2)	0.5459 (6)	0.87722 (9)	0.1199 (11)
O3	0.3379 (2)	0.8260 (5)	0.91548 (8)	0.1118 (10)
C1	0.3993 (3)	0.4150 (7)	0.56360 (11)	0.0898 (12)
C2	0.3295 (3)	0.3823 (7)	0.58702 (11)	0.0857 (11)
H2	0.2876	0.2765	0.5807	0.103*
C3	0.3223 (2)	0.5087 (6)	0.62015 (10)	0.0757 (10)
H3	0.2749	0.4882	0.6362	0.091*
C4	0.3841 (2)	0.6647 (6)	0.62979 (10)	0.0619 (8)
C5	0.4538 (3)	0.6952 (7)	0.60590 (11)	0.0824 (11)
H5	0.4959	0.8008	0.6120	0.099*
C6	0.4606 (3)	0.5678 (8)	0.57284 (12)	0.1048 (14)
H6	0.5079	0.5872	0.5567	0.126*
C7	0.4336 (2)	0.9377 (6)	0.67551 (10)	0.0679 (9)
H7A	0.4406	1.0551	0.6564	0.082*
H7B	0.4886	0.8629	0.6790	0.082*
C8	0.40363 (19)	1.0367 (5)	0.71267 (10)	0.0596 (8)
C9	0.41060 (19)	0.9171 (5)	0.74654 (10)	0.0588 (8)
H9	0.4367	0.7761	0.7462	0.071*
C10	0.37953 (19)	1.0021 (5)	0.78124 (10)	0.0573 (8)
C11	0.3427 (2)	1.2169 (5)	0.78140 (11)	0.0649 (9)
H11	0.3227	1.2787	0.8043	0.078*
C12	0.3361 (2)	1.3359 (6)	0.74792 (11)	0.0711 (9)
H12	0.3110	1.4781	0.7481	0.085*

C13	0.3661 (2)	1.2477 (6)	0.71394 (12)	0.0702 (9)
H13	0.3612	1.3313	0.6914	0.084*
C14	0.3823 (2)	0.8606 (6)	0.81570 (10)	0.0678 (9)
H14	0.4047	0.7168	0.8122	0.081*
C15	0.3574 (2)	0.9096 (6)	0.85094 (10)	0.0782 (10)
H15	0.3378	1.0539	0.8566	0.094*
C16	0.3602 (2)	0.7391 (8)	0.88138 (12)	0.0839 (11)
C17	0.3380 (4)	0.6729 (10)	0.94758 (13)	0.1363 (19)
H17A	0.2947	0.5598	0.9437	0.204*
H17B	0.3259	0.7545	0.9708	0.204*
H17C	0.3935	0.6024	0.9496	0.204*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.2067 (8)	0.1611 (7)	0.0952 (5)	−0.0426 (5)	0.0403 (4)	−0.0565 (4)
O1	0.0677 (14)	0.0822 (16)	0.0602 (14)	−0.0103 (13)	0.0043 (11)	−0.0070 (12)
O2	0.153 (3)	0.111 (2)	0.095 (2)	0.054 (2)	0.0227 (19)	0.028 (2)
O3	0.146 (3)	0.125 (2)	0.0641 (18)	0.019 (2)	0.0085 (17)	0.0156 (17)
C1	0.122 (3)	0.083 (3)	0.065 (2)	−0.012 (3)	0.011 (2)	−0.012 (2)
C2	0.101 (3)	0.086 (3)	0.070 (2)	−0.020 (2)	−0.002 (2)	−0.003 (2)
C3	0.073 (2)	0.093 (3)	0.061 (2)	−0.012 (2)	0.0019 (17)	−0.004 (2)
C4	0.068 (2)	0.066 (2)	0.051 (2)	0.0013 (18)	−0.0010 (16)	0.0095 (17)
C5	0.089 (3)	0.091 (3)	0.067 (2)	−0.016 (2)	0.012 (2)	−0.002 (2)
C6	0.120 (3)	0.117 (4)	0.077 (3)	−0.024 (3)	0.032 (2)	−0.014 (3)
C7	0.068 (2)	0.071 (2)	0.065 (2)	−0.0073 (18)	0.0012 (16)	0.0018 (18)
C8	0.0560 (19)	0.058 (2)	0.064 (2)	−0.0026 (16)	−0.0043 (15)	−0.0005 (17)
C9	0.0608 (19)	0.0459 (18)	0.070 (2)	0.0039 (15)	−0.0045 (16)	−0.0035 (17)
C10	0.0540 (18)	0.054 (2)	0.064 (2)	0.0023 (15)	−0.0053 (15)	−0.0004 (17)
C11	0.064 (2)	0.056 (2)	0.074 (2)	0.0021 (16)	0.0009 (17)	−0.0127 (18)
C12	0.075 (2)	0.0505 (19)	0.088 (3)	0.0072 (17)	−0.002 (2)	0.007 (2)
C13	0.074 (2)	0.062 (2)	0.075 (3)	−0.0012 (19)	−0.0049 (19)	0.0131 (19)
C14	0.070 (2)	0.070 (2)	0.064 (2)	0.0064 (18)	−0.0031 (17)	−0.0047 (19)
C15	0.090 (3)	0.076 (2)	0.068 (2)	0.017 (2)	−0.001 (2)	0.003 (2)
C16	0.080 (3)	0.104 (3)	0.067 (3)	0.021 (2)	0.003 (2)	0.009 (2)
C17	0.165 (5)	0.167 (5)	0.077 (3)	0.014 (4)	0.009 (3)	0.034 (3)

Geometric parameters (Å, º)

Br1—C1	1.902 (4)	C9—H9	0.9300
C1—C6	1.355 (6)	C10—C11	1.398 (4)
C1—C2	1.369 (5)	C10—C14	1.464 (5)
C2—C3	1.380 (5)	C11—C12	1.366 (5)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.375 (5)	C12—C13	1.374 (5)
C3—H3	0.9300	C12—H12	0.9300
C4—O1	1.367 (4)	C13—H13	0.9300
C4—C5	1.376 (5)	C14—C15	1.317 (4)

C5—C6	1.380 (5)	C14—H14	0.9300
C5—H5	0.9300	C15—C16	1.466 (5)
C6—H6	0.9300	C15—H15	0.9300
C7—O1	1.431 (4)	C16—O2	1.196 (4)
C7—C8	1.494 (5)	C16—O3	1.339 (5)
C7—H7A	0.9700	C17—O3	1.440 (5)
C7—H7B	0.9700	C17—H17A	0.9600
C8—C9	1.380 (5)	C17—H17B	0.9600
C8—C13	1.382 (4)	C17—H17C	0.9600
C9—C10	1.394 (4)		

C6—C1—C2	120.7 (4)	C9—C10—C11	118.4 (3)
C6—C1—Br1	120.9 (3)	C9—C10—C14	119.3 (3)
C2—C1—Br1	118.4 (3)	C11—C10—C14	122.2 (3)
C1—C2—C3	118.9 (4)	C12—C11—C10	120.0 (3)
C1—C2—H2	120.5	C12—C11—H11	120.0
C3—C2—H2	120.5	C10—C11—H11	120.0
C4—C3—C2	120.9 (3)	C11—C12—C13	120.7 (3)
C4—C3—H3	119.6	C11—C12—H12	119.7
C2—C3—H3	119.6	C13—C12—H12	119.7
O1—C4—C3	115.5 (3)	C12—C13—C8	121.0 (3)
O1—C4—C5	125.2 (3)	C12—C13—H13	119.5
C3—C4—C5	119.4 (3)	C8—C13—H13	119.5
C4—C5—C6	119.4 (4)	C15—C14—C10	128.7 (3)
C4—C5—H5	120.3	C15—C14—H14	115.6
C6—C5—H5	120.3	C10—C14—H14	115.6
C1—C6—C5	120.7 (4)	C14—C15—C16	120.7 (4)
C1—C6—H6	119.7	C14—C15—H15	119.6
C5—C6—H6	119.7	C16—C15—H15	119.6
O1—C7—C8	107.5 (3)	O2—C16—O3	122.9 (4)
O1—C7—H7A	110.2	O2—C16—C15	125.7 (4)
C8—C7—H7A	110.2	O3—C16—C15	111.4 (4)
O1—C7—H7B	110.2	O3—C17—H17A	109.5
C8—C7—H7B	110.2	O3—C17—H17B	109.5
H7A—C7—H7B	108.5	H17A—C17—H17B	109.5
C9—C8—C13	118.2 (3)	O3—C17—H17C	109.5
C9—C8—C7	120.7 (3)	H17A—C17—H17C	109.5
C13—C8—C7	121.0 (3)	H17B—C17—H17C	109.5
C8—C9—C10	121.7 (3)	C4—O1—C7	117.9 (2)
C8—C9—H9	119.2	C16—O3—C17	116.3 (4)
C10—C9—H9	119.2		

C6—C1—C2—C3	0.4 (6)	C9—C10—C11—C12	1.4 (5)
Br1—C1—C2—C3	178.9 (3)	C14—C10—C11—C12	−175.3 (3)
C1—C2—C3—C4	−0.3 (6)	C10—C11—C12—C13	−0.6 (5)
C2—C3—C4—O1	−180.0 (3)	C11—C12—C13—C8	0.1 (5)
C2—C3—C4—C5	0.3 (5)	C9—C8—C13—C12	−0.4 (5)
O1—C4—C5—C6	179.9 (3)	C7—C8—C13—C12	178.0 (3)

C3—C4—C5—C6	−0.4 (6)	C9—C10—C14—C15	179.2 (3)
C2—C1—C6—C5	−0.5 (7)	C11—C10—C14—C15	−4.1 (5)
Br1—C1—C6—C5	−179.0 (3)	C10—C14—C15—C16	176.0 (3)
C4—C5—C6—C1	0.5 (6)	C14—C15—C16—O2	−4.0 (7)
O1—C7—C8—C9	77.1 (3)	C14—C15—C16—O3	175.8 (3)
O1—C7—C8—C13	−101.2 (3)	C3—C4—O1—C7	177.7 (3)
C13—C8—C9—C10	1.2 (4)	C5—C4—O1—C7	−2.7 (5)
C7—C8—C9—C10	−177.1 (3)	C8—C7—O1—C4	−179.2 (3)
C8—C9—C10—C11	−1.8 (4)	O2—C16—O3—C17	−0.5 (6)
C8—C9—C10—C14	175.1 (3)	C15—C16—O3—C17	179.7 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O2^{i}	0.93	2.45	3.370 (6)	172
C12—H12···*Cg*2^{ii}	0.93	2.99	3.677 (3)	132

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) *x*, −*y*−1/2, *z*−1/2.