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Methyl {2-[3-(4-bromophenyl)-1,2,4-oxadiazol-5-ylmethoxy]phenyl}acetate

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Key indicators

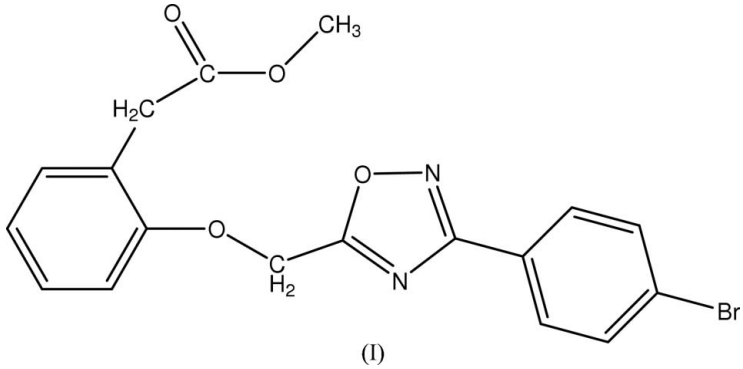
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.046
wR factor = 0.142
Data-to-parameter ratio = 13.4

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

The title compound, $C_{18}H_{15}BrN_2O_4$, was synthesized by the reaction of methyl (2-hydroxyphenyl)acetate and 3-(4-bromo)phenyl-5-chloromethyl-1,2,4-oxadiazole. Weak intramolecular C—H···N hydrogen bonds are observed in the crystal structure.

Comment

1,2,4-Oxadiazole derivatives are of great interest because of their biological properties. Some derivatives of 1,2,4-oxadiazole have intrinsic analgesic (Terashita *et al.*, 2002), anti-inflammatory (Nicolaides *et al.*, 1998) and anti-picornaviral (Romero, 2001) properties and show high efficacy as agonists [*e.g.* for muscarinic (Macor *et al.*, 1996), adrenergic (Quagliato & Andrae, 2002) and 5-hydroxytryptamine (Gur *et al.*, 2001)] and antagonists [*e.g.* for angiotensin (Naka & Kubo, 1999) and adhesion (Juraszyk *et al.*, 1997)] for different receptors. We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1 in which dashed lines indicate intramolecular C—H···N hydrogen bonds (Table 2). The bond lengths and angles are given in Table 1.

Experimental

Methyl (2-hydroxyphenyl)acetate (20 mmol) was dissolved in acetone (20 ml) and potassium carbonate (30 mmol) was added in one portion. 3-(4-Bromophenyl)-5-chloromethyl-1,2,4-oxadiazole (20 mmol) in acetone (20 ml) was added to this mixture. The resulting mixture was refluxed for 6 h, then concentrated under reduced pressure to afford crude (I). Pure (I) was obtained by recrystallization from ethyl acetate. Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution. ^{1}H NMR ($CDCl_3$): δ 7.94–7.97 (*m*, 2H), 7.61–7.63 (*m*, 2H), 7.23–7.29 (*m*, 2H), 6.97–7.03 (*m*, 2H), 5.35 (*s*, 2H), 3.72 (*s*, 2H), 3.69 (*s*, 3H).

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Crystal data

$C_{18}H_{15}BrN_2O_4$
M_r = 403.23
Monoclinic, $C2/c$
a = 20.011 (4) Å
b = 9.643 (2) Å
c = 18.089 (4) Å
β = 98.33 (3)°
V = 3453.7 (12) Å^3
Z = 8
D_x = 1.551 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 9–12°
μ = 2.41 mm^{-1}
T = 293 (2) K
Block, colourless
0.40 × 0.40 × 0.20 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.446, T_{max} = 0.645
3130 measured reflections
3038 independent reflections
1670 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.0°
$h = 0 \rightarrow 23$
$k = 0 \rightarrow 11$
$l = -21 \rightarrow 21$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.142
S = 1.02
3038 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 0.6P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0030 (3)

Table 1
Selected geometric parameters (Å, °).

Br—C16	1.898 (5)	N1—C11	1.287 (6)
O1—C2	1.333 (6)	N1—C12	1.375 (6)
O1—C1	1.441 (6)	N2—C12	1.310 (6)
O2—C2	1.187 (5)	C2—C3	1.496 (7)
O3—C9	1.382 (6)	C3—C4	1.499 (7)
O3—C10	1.405 (6)	C10—C11	1.474 (7)
O4—C11	1.333 (6)	C12—C13	1.467 (6)
O4—N2	1.416 (5)		
C2—O1—C1	116.2 (4)	O3—C10—C11	108.8 (4)
C9—O3—C10	117.7 (4)	N1—C11—O4	113.8 (5)
C11—O4—N2	106.3 (3)	N1—C11—C10	128.0 (5)
C11—N1—C12	102.7 (4)	O4—C11—C10	118.2 (4)
C12—N2—O4	102.7 (4)	N2—C12—N1	114.5 (4)
O2—C2—O1	123.1 (5)	N2—C12—C13	122.1 (5)
O2—C2—C3	125.3 (5)	N1—C12—C13	123.5 (4)
O1—C2—C3	111.6 (4)	C18—C13—C12	122.0 (4)
C2—C3—C4	112.9 (4)	C14—C13—C12	119.0 (5)
O3—C9—C4	114.1 (4)	C15—C16—Br	119.0 (4)
O3—C9—C8	124.6 (5)	C17—C16—Br	120.5 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14A···N1	0.93	2.57	2.899 (7)	101
C18—H18A···N2	0.93	2.60	2.889 (7)	100

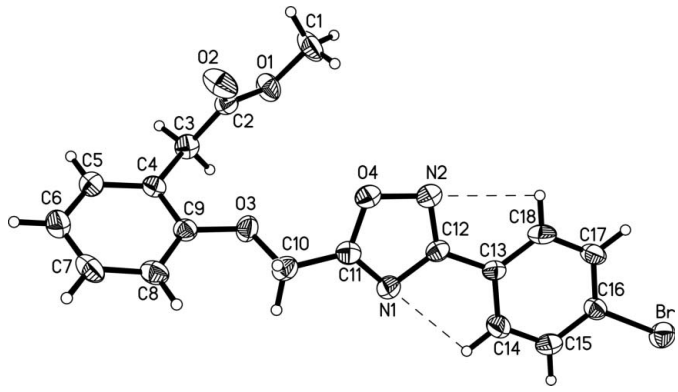

Figure 1
A view of the molecular structure of (I), with dashed lines indicating intramolecular C—H···N hydrogen bonds. Displacement ellipsoids are drawn at the 30% probability level

All H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.97 Å. They were included in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

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