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Methyl 2-[3-(4-bromophenyl)-1,2,4-oxadiazol-5-ylmethoxy]phenylacetate

Zhi-Qian Liu, Zhi-Qian Liu, Xiao-Chen Yan and Hai-Bo Wang*

Department of Applied Chemistry, College of Science, Nanjing University of Technolgy, Xinmofan Road No. 5, Nanjing 210009, People's Republic of China

Correspondence e-mail: wanghaibo@njut.edu.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.109
wR factor = 0.209
Data-to-parameter ratio = 14.0

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

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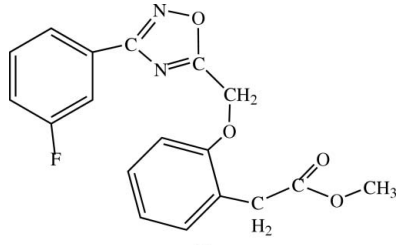
The title compound, $C_{18}H_{15}FN_2O_4$, was synthesized by the reaction of methyl (2-hydroxyphenyl)acetate and 3-(4-bromo)phenyl-5-chloromethyl-1,2,4-oxadiazole. Weak intramolecular C—H···N hydrogen bonds are observed in the crystal structure.

Comment

1,2,4-Oxadiazole derivatives are of great interest because of their biological properties. Some derivatives of 1,2,4-oxadiazoles 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 receptors (Gur *et al.*, 2001)] and antagonists [*e.g.* for angiotensin (Naka & Kubo, 1999) and adhesion receptors (Juraszyk *et al.*, 1997)]. We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. 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-Fluorophenyl)-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 and then concentrated under reduced pressure to afford crude compound (I). Pure compound (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.

Crystal data

$C_{18}H_{15}FN_2O_4$
M_r = 342.32
Monoclinic, $P2_1/c$
a = 11.603 (2) Å
b = 9.0170 (18) Å
c = 15.692 (3) Å
β = 96.90 (3)°
V = 1629.9 (6) Å^3
Z = 4
D_x = 1.395 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.969, T_{max} = 0.989
3165 measured reflections
3165 independent reflections
1291 reflections with $I > 2\sigma(I)$
R_{int} = 0.000
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.109
$wR(F^2)$ = 0.209
S = 1.05
3165 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.01P)^2 + 5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

F—C16	1.378 (7)	O4—C11	1.345 (7)
O1—C2	1.338 (6)	O4—N1	1.403 (6)
O1—C1	1.430 (6)	N1—C12	1.315 (8)
O2—C2	1.200 (6)	N2—C11	1.295 (6)
O3—C9	1.408 (7)	N2—C12	1.355 (7)
O3—C10	1.445 (8)		
C2—O1—C1	116.3 (4)	O3—C10—C11	112.3 (6)
C9—O3—C10	116.0 (5)	N2—C11—O4	111.1 (5)
C11—O4—N1	107.6 (5)	N2—C11—C10	134.6 (6)
C12—N1—O4	102.6 (5)	O4—C11—C10	114.1 (6)
C11—N2—C12	104.6 (5)	N1—C12—N2	114.1 (5)
O2—C2—O1	122.5 (5)	N1—C12—C13	122.0 (6)
O2—C2—C3	124.6 (5)	N2—C12—C13	123.9 (6)
O1—C2—C3	112.7 (5)	C17—C16—F	117.7 (9)
C8—C9—O3	126.4 (7)	F—C16—C15	118.2 (8)
C4—C9—O3	111.1 (6)		

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

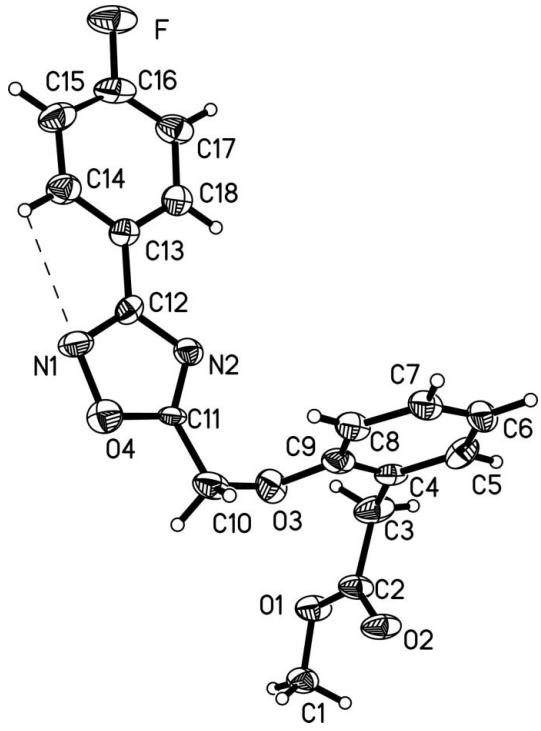


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. The dashed line indicates the intramolecular C—H···N hydrogen bond.

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