Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Methyl 2-{[3-(2-methyl)phenyl-1,2,4-oxadiazol-5-yl]methoxy}phenylacetate

Hai-Bo Wang,* Yue-Qing Pu, Jia-Hui Chen and Jin-Tang Wang

Department of Applied Chemistry, College of Science, Nanjing University of Technolgy, Xinmofan Road No.5 Nanjing, 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) = 0.004 Å
R factor = 0.055
wR factor = 0.168
Data-to-parameter ratio = 14.8

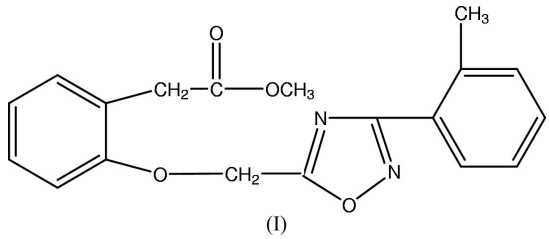
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 1 April 2005
Accepted 13 April 2005
Online 23 April 2005

The title compound, $C_{19}H_{18}N_2O_4$, was synthesized by the reaction of methyl (2-hydroxyphenyl)acetate and 3-(2-methyl)phenyl-5-chloromethyl-1,2,4-oxadiazole. C—H···N-type hydrogen bonds are observed in the molecular structure. In the crystal structure, there are weak intermolecular C—H···O hydrogen bonds and C—H···π interactions.

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-hydroxy-tryptamine (Gur *et al.*, 2001)] and antagonists [*e.g.* for angiotensin (Naka & Kubo, 1999) and adhesion agents (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, and selected bond lengths and bond angles are given in Table 1. The C4–C9 and C13–C18 benzene rings form dihedral angles

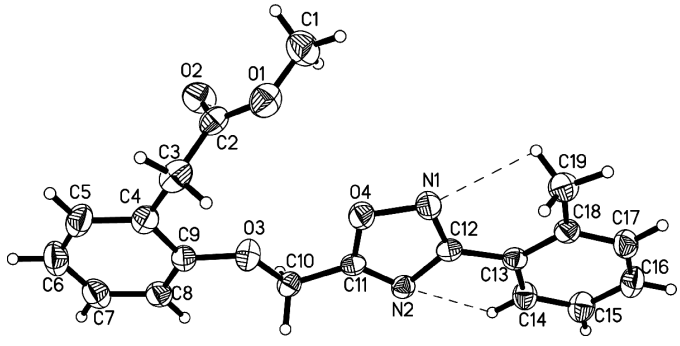


Figure 1
A view of the molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. Hydrogen bonds are shown as dashed lines.

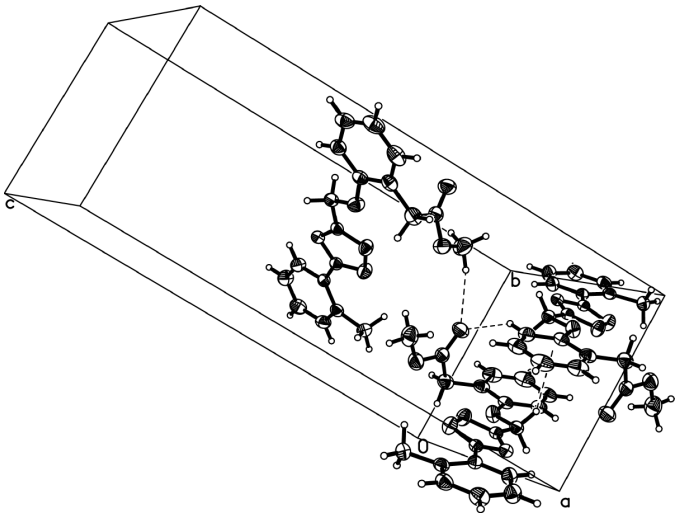


Figure 2
The short C—H···O and C—H···π interactions (dashed lines) in the crystal structure of (I).

of 11.3 (2) and 13.7 (1)°, respectively, with the oxadiazole ring.

In the molecular structure, C—H···N type hydrogen bonds are observed. In the crystal structure, the molecules are linked by C—H···O hydrogen bonds and C—H···π interactions (Table 2 and Fig. 2), leading to the formation of a three-dimensional network.

Experimental

Methyl (2-hydroxyphenyl)acetate (20 mmol) was dissolved in acetone (20 ml) and potassium carbonate (30 mmol) was added in one portion. 3-(2-Methyl)phenyl-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 (m.p. 339–341 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution. Spectroscopic analysis: ^{1}H NMR ($CDCl_3$, δ, p.p.m.): 7.99–8.00 (*m*, 1H), 7.37–7.39 (*m*, 1H), 7.31–7.32 (*m*, 2H), 7.23–7.29 (*m*, 2H), 6.99–7.03 (*m*, 2H), 5.37 (*s*, 2H), 3.74 (*s*, 2H), 3.69 (s, 3H), 2.62 (*s*, 3H).

Crystal data

$C_{19}H_{18}N_2O_4$
M_r = 338.35
Monoclinic, $P2_1/c$
a = 11.444 (2) Å
b = 7.9540 (16) Å
c = 19.356 (4) Å
β = 102.83 (3)°
V = 1717.9 (6) Å^3
Z = 4
D_x = 1.308 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 9–12°
μ = 0.09 mm^{-1}
T = 293 (2) K
Rod, colourless
0.40 × 0.20 × 0.20 mm

Data collection

Enraf-Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
3535 measured reflections
3361 independent reflections
1923 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 26.0°
$h = 0 \rightarrow 14$
$k = 0 \rightarrow 9$
$l = -23 \rightarrow 23$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.168
S = 1.03
3361 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.08P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.014 (2)

Table 1
Selected geometric parameters (Å, °).

O1—C2	1.324 (3)	N2—C11	1.282 (3)
O1—C1	1.437 (4)	N2—C12	1.386 (3)
O2—C2	1.210 (3)	C2—C3	1.498 (4)
O3—C9	1.381 (3)	C3—C4	1.502 (4)
O3—C10	1.405 (3)	C10—C11	1.483 (3)
O4—C11	1.329 (3)	C12—C13	1.470 (3)
O4—N1	1.418 (3)	C18—C19	1.497 (4)
N1—C12	1.297 (3)		
C2—O1—C1	116.9 (3)	O3—C9—C4	114.2 (2)
C9—O3—C10	119.53 (19)	O3—C10—C11	107.0 (2)
C11—O4—N1	105.99 (18)	N2—C11—O4	114.0 (2)
C12—N1—O4	103.4 (2)	N2—C11—C10	127.8 (2)
C11—N2—C12	102.8 (2)	O4—C11—C10	118.2 (2)
O2—C2—O1	123.0 (3)	N1—C12—N2	113.8 (2)
O2—C2—C3	124.1 (3)	N1—C12—C13	124.4 (2)
O1—C2—C3	112.9 (3)	N2—C12—C13	121.8 (2)
C2—C3—C4	113.0 (2)	C14—C13—C12	116.8 (2)
C9—C4—C3	119.5 (2)	C18—C13—C12	123.8 (2)
C5—C4—C3	123.3 (3)	C17—C18—C19	118.7 (3)
C8—C9—O3	124.1 (2)	C13—C18—C19	124.2 (2)

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

*Cg*1 is the centroid of the C4–C9 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1*B*···O2^{i}	0.96	2.53	3.480 (4)	169
C8—H8*A*···O2^{ii}	0.93	2.54	3.365 (3)	149
C14—H14*A*···N2	0.93	2.47	2.839 (3)	104
C19—H19*C*···N1	0.96	2.54	2.880 (4)	101
C10—H10*A*···*Cg*1^{ii}	0.97	2.82	3.592 (3)	138

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

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) = 1.2 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*.

References

Enraf-Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf-Nonius, Delft, The Netherlands.
Gur, E., Dremencov, E., Lerer, B. & Newman, M. E. (2001). *Eur. J. Pharmacol.* **411**, 115–122.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.

Juraszyk, H., Gante, J., Wurziger, H., Bernotat-Danielowski, S. & Melzer, G. (1997). PCT Int. Appl. No. 9744333.
Macor, J. E., Ordway, T., Smith, R. L., Verhoest, P. R. & Mack, R. A. (1996). *J. Org. Chem.* **61**, 3228–3229.
Naka, T. & Kubo, K. (1999). *Curr. Pharm. Des.* **5**, 453–472.
Nicolaides, D. N., Fylaktakidou, K. C., Litinas, K. E. & Hadjipavlou-Litina, D. (1998). *Eur. J. Med. Chem.* **33**, 715–724.
Quagliato, D. A. & Andrae, P. M. (2002). PCT Int. Appl. WO, 0206250.
Romero, J. R. (2001). *Expert Opin. Invest. Drugs*, **10**, 369–379.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Siemens (1996). *SHELXTL*. Version 5.06. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Terashita, Z., Naruo, K. & Morimoto, S. (2002). PCT Int. Appl. WO, 0260439.