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

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Key indicators

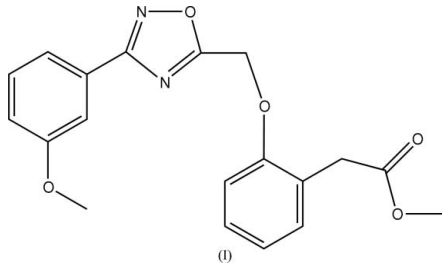
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.064
wR factor = 0.170
Data-to-parameter ratio = 14.7

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

The title compound, $C_{19}H_{18}N_2O_5$, was synthesized by the reaction of methyl (2-hydroxyphenyl)acetate and 5-chloromethyl-3-(3-methoxyphenyl)-1,2,4-oxadiazole. The plane of the oxadiazole ring forms a small dihedral angle of 15.2 (2)° with the plane of the benzene ring directly bonded to it, whereas the second benzene ring is approximately orthogonal to the oxadiazole plane, the dihedral angle being 79.1 (2)°.

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 or antagonists for different receptors [*e.g.* agonists for muscarinic (Macor *et al.*, 1996), adrenergic (Quagliato & Andrae, 2002), 5-hydroxytryptamine (Gur *et al.*, 2001) and antagonists for angiotensin (Naka & Kubo, 1999) and adhesion (Juraszyk *et al.*, 1997) receptors]. We are focusing our synthetic and structural studies on 1,2,4-oxadiazole derivatives and recently published the structure of methyl {2-[(3-phenyl-1,2,4-oxadiazol-5-yl)methoxy]phenyl}acetate (Wang *et al.*, 2004). In the present paper, we report the structure of its close analogue, (I), which has a *p*-methoxyphenyl group instead of an unsubstituted phenyl substituent.



(I)

The plane of the oxadiazole ring in (I) (Fig. 1) forms a small dihedral angle of 15.2 (2)° with the plane of the benzene ring (C2–C7) directly bonded to it. The plane of the second benzene ring (C11–C16) is almost orthogonal to the oxadiaole plane, forming a dihedral angle of 79.1 (2)°.

Experimental

Methyl (2-hydroxyphenyl)acetate (20 mmol) was dissolved in acetone (20 ml). Potassium carbonate (30 mmol) was then added to this solution in one portion. 5-Chloromethyl-3-(3-methoxyphenyl)-1,2,4-oxadiazole (20 mmol) in acetone (20 ml) was added to the mixture which was then refluxed for 6 h and finally 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 studies were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{19}H_{18}N_2O_5$
M_r = 354.35
Monoclinic, $P2_1/n$
a = 8.9620 (18) Å
b = 7.9500 (16) Å
c = 25.021 (5) Å
β = 96.51 (3)°
V = 1771.2 (6) Å^3
Z = 4
D_x = 1.329 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 9–12°
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, colourless
0.40 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.962, T_{max} = 0.990
3695 measured reflections
3465 independent reflections
1935 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 26.0°
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 9$
$l = -30 \rightarrow 30$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.170
S = 1.03
3465 reflections
236 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 0.02P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0095 (17)

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.416 (5)	O4—C18	1.330 (4)
O1—C2	1.357 (4)	O4—C19	1.459 (4)
O2—N2	1.428 (3)	O5—C18	1.188 (3)
O2—C9	1.322 (3)	N1—C8	1.382 (4)
O3—C10	1.413 (3)	N1—C9	1.290 (4)
O3—C11	1.388 (3)	N2—C8	1.297 (4)
C2—O1—C1	118.5 (3)	N1—C8—C4	123.3 (3)
C9—O2—N2	106.3 (2)	N1—C9—O2	114.0 (3)
C11—O3—C10	118.5 (2)	N1—C9—C10	130.3 (3)
C18—O4—C19	115.1 (3)	O2—C9—C10	115.7 (3)
C9—N1—C8	102.3 (2)	O3—C10—C9	112.3 (2)
C8—N2—O2	102.5 (2)	O5—C18—O4	124.4 (3)
N2—C8—N1	114.8 (3)	O5—C18—C17	124.5 (3)
N2—C8—C4	121.9 (3)	O4—C18—C17	111.0 (3)

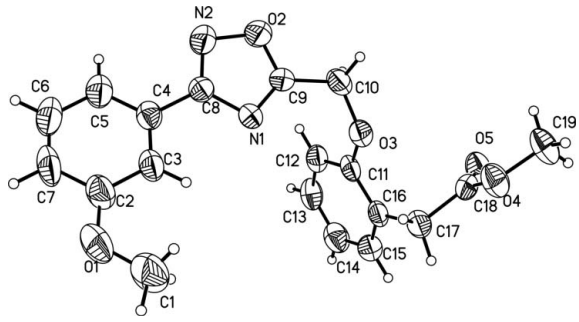


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

All H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.97 Å. They were refined 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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