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

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Key indicators

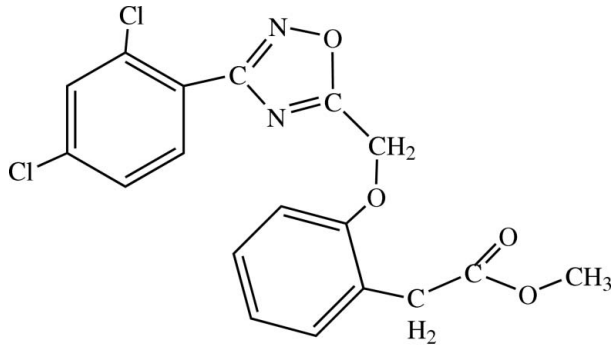
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.069
wR factor = 0.178
Data-to-parameter ratio = 14.8

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

The geometrical parameters for the title compound, $C_{18}H_{14}Cl_2N_2O_4$, are normal. The torsion angle between the oxadiazole ring and its attached benzene ring is 25.4 (2)°.

Comment

1,2,4-Oxadiazole derivatives are of great interest because of their biological effects, such as anti-inflammatory (Nicolaides *et al.*, 1998), and antipicornaviral (Romero, 2001) properties. As part of our studies of these compounds, we report here the crystal structure of the title compound, (I) (Fig. 1).



(I)

The geometrical paramaters for (I) are normal. The mean plane of the oxadiazole ring (C11/C12/N1/N2/O4) is almost coplanar with the mean plane of the C4–C9 benzene ring [dihedral angle = 2.3 (2)°]. Conversely, the mean plane of the C13–C18 benzene ring is distinctly twisted with respect to the oxadiazole ring [dihedral angle = 25.4 (2)°] perhaps as a result of steric repulsion between N2 and Cl1 [separation = 3.050 (4) Å; van der Waals contact distance = 3.30 Å].

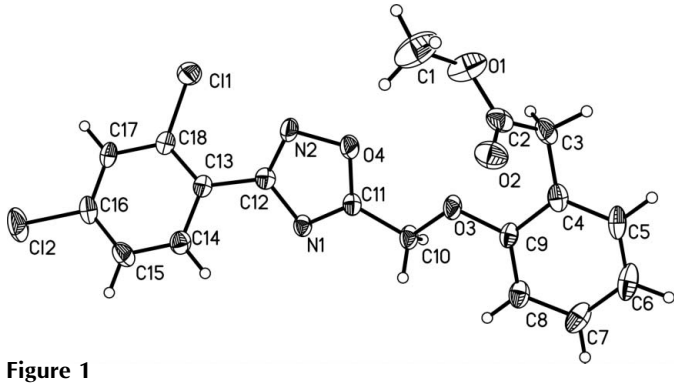


Figure 1
A view of the molecular structure of (I), showing 30% displacement ellipsoids (arbitrary spheres for the H atoms).

Experimental

Methyl (2-hydroxyphenyl)acetate (20 mmol) was dissolved in acetone (20 ml) and potassium carbonate (30 mmol) was added in one portion. 5-Chloromethyl-3-(2,4-chlorophenyl)-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 the crude product. 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

$C_{18}H_{14}Cl_2N_2O_4$
$M_r = 393.21$
Monoclinic, $P2_1/c$
$a = 7.4910\ (15)$ Å
$b = 15.613\ (3)$ Å
$c = 15.100\ (3)$ Å
$\beta = 90.59\ (3)^\circ$
$V = 1766.0\ (6)$ Å^3
$Z = 4$
$D_x = 1.479$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.39$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
0.30 × 0.10 × 0.10 mm

Data collection

Nonius CAD4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.891$, $T_{max} = 0.962$
3737 measured reflections
3467 independent reflections
1958 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 26.0^\circ$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.069$
$wR(F^2) = 0.178$
$S = 1.04$
3467 reflections
235 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.076P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

All H atoms were placed in calculated positions, with C—H = 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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