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2-[3-(4-Methylphenyl)-1,2,4-oxadiazol-5-yl]phenol

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.063
wR factor = 0.181
Data-to-parameter ratio = 7.9

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

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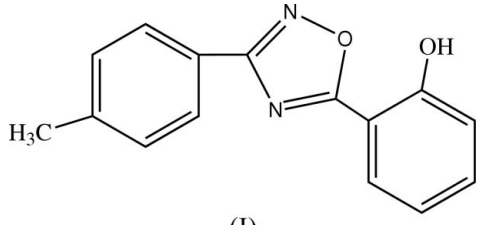
In the approximately planar molecule of the title compound, $C_{15}H_{12}N_2O_2$, which is a derivative of oxadiazole, an intramolecular O—H···N hydrogen bond helps to establish the molecular conformation.

Comment

As part of our onging structural studies of 1,2,4-oxadiazole derivatives (Ding *et al.*, 2006), we report here the synthesis and crystal structure of the title compound, (I) (Fig. 1).



(I)

The dihedral angles between the N2/C9/O1/N1/C8 ring and its adjacent benzene rings are 3.9 (3) and 5.0 (3)° for the C10 and C5 rings, respectively. An intramolecular O—H···N hydrogen bond (Table 1) helps to establish the molecular conformation of (I).

Experimental

4-Methylbenzoic acid amidoxime (50 mmol) and methyl salicylate (100 mmol) were dissolved in anhydrous ethanol (150 ml) mixed with sodium (2.3 g) and heated for 3 × 25 min (with a 5 min break each time) at 400 W in a microwave. The reaction mixture was then concentrated by evaporation *in vacuo* to about one-third of its volume and the residue was mixed with water (20 ml). Whilst cooling the mixture, the pH was adjusted to 8–9 with 2 *M* hydrochloric acid, and the resulting precipitate was recovered by suction filtration and washed with water. In order to remove all traces of water, the compound was then dissolved in dichloromethane, dried with sodium sulfate and concentrated by evaporation. Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{15}H_{12}N_2O_2$
M_r = 252.27
Monoclinic, $P2_1$
a = 6.5110 (13) Å
b = 5.172 (1) Å
c = 18.763 (4) Å
β = 99.14 (3)°
V = 623.8 (2) Å^3
Z = 2
D_x = 1.343 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 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} = 0.973, T_{max} = 0.991
1483 measured reflections
1360 independent reflections
900 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.181
S = 1.06
1360 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.099P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···N2	0.82	1.94	2.663 (5)	147

Due to insignificant anomalous scattering, Friedel pairs were merged before refinement. All H atoms were positioned geometrically, with N—H = 0.86 Å and C—H = 0.93–0.96 Å, and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C,N) 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: *PLATON* (Spek, 2003).

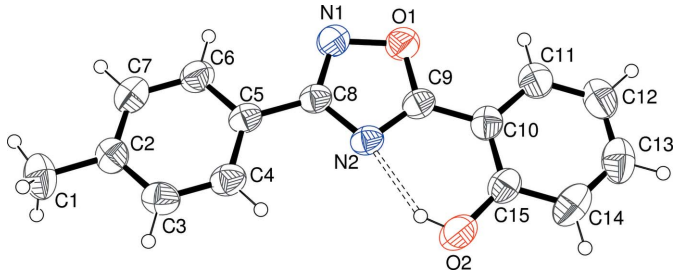


Figure 1
A view of the molecular structure of (I), showing 40% probability displacement ellipsoids (arbitrary spheres for the H atoms). The dashed lines indicate the hydrogen bond.

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