organic papers

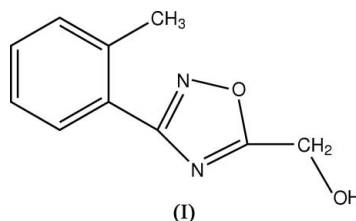# [3-(2-Methylphenyl)-1,2,4-oxadiazol-5-yl]-methanol

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

Department of Applied Chemistry, College of Science, Nanjing University of Technology, 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 = 0.053
wR factor = 0.152
Data-to-parameter ratio = 13.8

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

The crystal structure of the title compound, $C_{10}H_{10}N_2O_2$, is characterized by an O—H···N hydrogen bond.

Comment

1,2,4-Oxadiazoles are important five-membered heterocycles. Some derivatives of 1,2,4-oxadiazoles have anti-inflammatory (Nicolaides *et al.*, 1998) and antipicornaviral (Romero, 2001) properties. The molecular structure of the title compound is shown in Fig. 1, with selected geometry in Table 1. The crystal structure is characterized by an O—H···N hydrogen bond (Table 2).

(I)

Experimental

Hexamethylenetetramine (90 mmol) was dissolved in acetic acid (70 ml) and water (70 mmol). 5-Chloromethyl-3-(2-methylphenyl)-1,2,4-oxadiazole (30 mmol) was added to this mixture. The resulting mixture was refluxed for 3 h. After cooling and filtering, crude (I) was obtained. Pure (I) was obtained by crystallization from a mixture of ethyl acetate (6 ml) and petrolum ether (6 ml). Crystals of (I) suitable for X-ray diffraction were obstained by slow evaporation of an ethanol solution.

Crystal data

$C_{10}H_{10}N_2O_2$	D_x = 1.389 Mg m^{-3}
M_r = 190.20	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 25
a = 7.529 (2) Å	reflections
b = 14.307 (3) Å	θ = 9–13°
c = 8.799 (3) Å	μ = 0.10 mm^{-1}
β = 106.39 (3)°	T = 293 (2) K
V = 909.3 (5) Å^3	Block, colourless
Z = 4	0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.019
$\omega/2\theta$ scans	θ_{max} = 26.0°
Absorption correction: ψ scan (North *et al.*, 1968)	$h = 0 \rightarrow 9$
	$k = 0 \rightarrow 17$
T_{min} = 0.971, T_{max} = 0.980	$l = -10 \rightarrow 10$
1896 measured reflections	3 standard reflections
1764 independent reflections	every 200 reflections
1242 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.08P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.053$	$+ 0.3P]$
$wR(F^2) = 0.152$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	$(\Delta/\sigma)_{max} = 0.002$
1764 reflections	$\Delta\rho_{max} = 0.14$ e Å^{-3}
128 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL97*
	Extinction coefficient: 0.0073 (10)

Table 1
Selected geometric parameters (Å, °).

O1—C9	1.331 (3)	N1—C8	1.302 (3)
O1—N1	1.414 (3)	N2—C9	1.285 (3)
O2—C10	1.404 (3)	N2—C8	1.378 (3)
C9—O1—N1	106.35 (17)	N2—C8—C7	121.91 (18)
C8—N1—O1	103.61 (17)	N2—C9—O1	113.1 (2)
C9—N2—C8	103.70 (18)	N2—C9—C10	129.1 (2)
N1—C8—N2	113.27 (19)	O1—C9—C10	117.8 (2)
N1—C8—C7	124.8 (2)	O2—C10—C9	110.3 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···N2^i	1.00	1.92	2.858 (3)	154

Symmetry code: (i) $-x + 1, -y + 1, -z + 3$.

All H atoms were positioned geometrically and refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C) or 1.5 U_{eq}(methyl C)] using a riding model with C—H = 0.93–0.97 Å. The O—H distance was set at 1.00 Å and the C—O torsion angle was refined.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms &
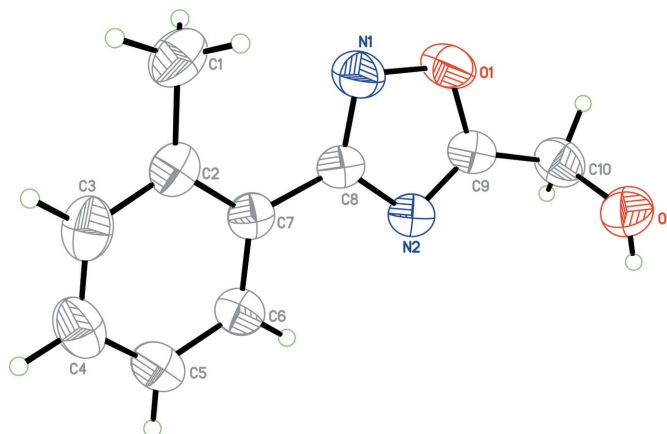

Figure 1
A view of the molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level.

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.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Nicolaides, D. N., Fylaktakidou, K. C., Litinas, K. E. & Hadjipavlou-Litina, D. (1998). *Eur. J. Med. Chem.* **33**, 715–724.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
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.