Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Methyl 3-(dimethylamino)-2-[2-(1-{3-[4-(methylsulfanyl)phenyl]-1,2,4-oxadiazol-5-yl}-2-(dimethylamino)vinyloxy)phenyl]acrylate

Hai-Bo Wang,* Jia-Hui Chen, Yue-Qing Pu 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) = 0.005 Å
R factor = 0.058
wR factor = 0.211
Data-to-parameter ratio = 15.5

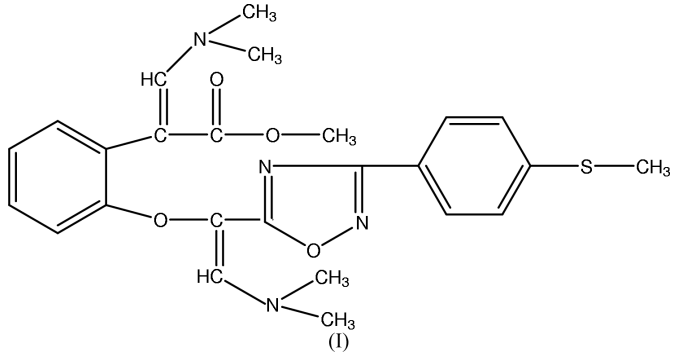
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_{25}H_{28}N_4O_4S$, which is a derivative of 1,2,4-oxadiazole, there are intramolecular C—H···O and intermolecular C—H···π interactions.

Received 19 November 2004
Accepted 2 December 2004
Online 11 December 2004

Comment

1,2,4-Oxadiazoles represent an important class of five-membered heterocycles. Some derivatives of 1,2,4-oxadiazoles have intrinsic analgesic (Terashita *et al.*, 2002), anti-inflammatory (Nicolaides *et al.*, 1998) and antipicornaviral (Romero, 2001) properties and are efficient as agonists [*e.g.* forangiotensin (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)

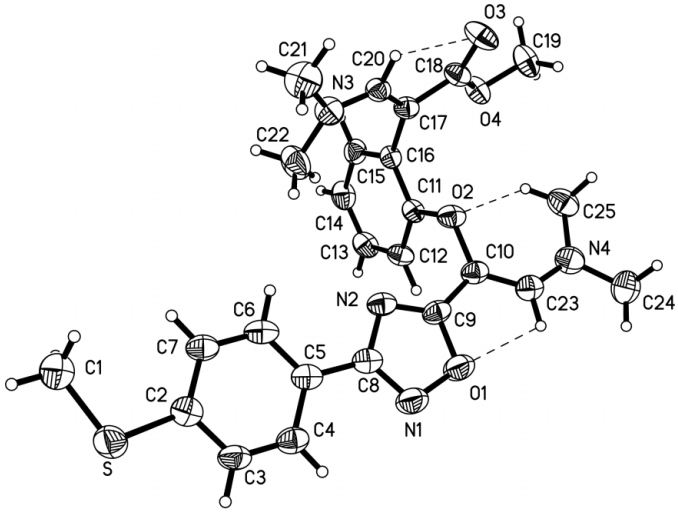


Figure 1
A view of the molecular structure of (I), showing displacement ellipsoids at the 30% probability level. Dashed lines indicate C—H···O hydrogen bonds.

The molecular structure of (I) is shown in Fig. 1, where the dashed lines indicate C—H···O hydrogen bonds (Table 2). There are also intermolecular C—H···π interactions (Fig. 2), *Cg*2 in Table 2 being the centroid of atoms C2–C7. The combination of C—H···O and C—H···π weak interactions generates a three-dimensional network.

Experimental

Methyl 2-({3-[4-(methylthio)phenyl]-1,2,4-oxadiazol-5-yl}methoxy)-phenylacetate (14 mmol) was dissolved in DMF (20 ml) and *N*,*N*-dimethylformamide dimethyl acetal (8 ml) was added in one portion. The resulting mixture was refluxed for 6 h and then concentrated under reduced pressure to afford crude compound (I) (yield 65%). Pure compound (I) was obtained by crystallizing from a mixture of ethyl acetate (15 ml) and petroleum ether (7.5 ml). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution. ^{1}H NMR ($CDCl_3$, p.p.m.): 7.87–7.88 (*m*, 2H), 7.69 (*m*, 1H), 7.31 (*m*, 1H), 7.25–7.27 (*m*, 2H), 7.16–7.18 (*m*, 2H), 6.93–6.94 (*m*, 1H), 6.86–6.88 (*m*, 1H), 3.55 (*s*, 3H), 3.00 (*s*, 6H), 2.84–2.86 (*m*, 6H), 2.50 (*s*, 3H).

Crystal data

$C_{25}H_{28}N_4O_4S$	D_x = 1.298 Mg m^{-3}
M_r = 480.57	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 25 reflections
a = 8.2940 (17) Å	θ = 9–13°
b = 12.654 (3) Å	μ = 0.17 mm^{-1}
c = 23.601 (5) Å	T = 293 (2) K
β = 97.02 (3)°	Block, colourless
V = 2458.4 (9) Å^3	0.4 × 0.3 × 0.3 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	θ_{max} = 26.0°
$\omega/2\theta$ scan	$h = 0 \rightarrow 9$
Absorption correction: none	$k = 0 \rightarrow 15$
5129 measured reflections	$l = -28 \rightarrow 28$
4785 independent reflections	3 standard reflections
2345 reflections with $I > 2\sigma(I)$	every 200 reflections
R_{int} = 0.057	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.058	$(\Delta/\sigma)_{max}$ = 0.009
$wR(F^2)$ = 0.211	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
S = 1.10	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
4785 reflections	Extinction correction: *SHELXL*97
308 parameters	Extinction coefficient: 0.0048 (13)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

S—C2	1.758 (4)	N1—C8	1.298 (5)
S—C1	1.781 (5)	N2—C9	1.297 (5)
O1—C9	1.344 (4)	N2—C8	1.390 (5)
O1—N1	1.419 (4)		
C9—O1—N1	106.4 (3)	N1—C8—N2	114.8 (4)
C8—N1—O1	103.1 (3)	N2—C9—O1	113.3 (4)
C9—N2—C8	102.4 (3)		
O1—N1—C8—N2	−1.4 (4)	C11—O2—C10—C9	−81.8 (4)
C4—C5—C8—N1	−11.6 (5)	C11—C16—C17—C18	86.8 (4)

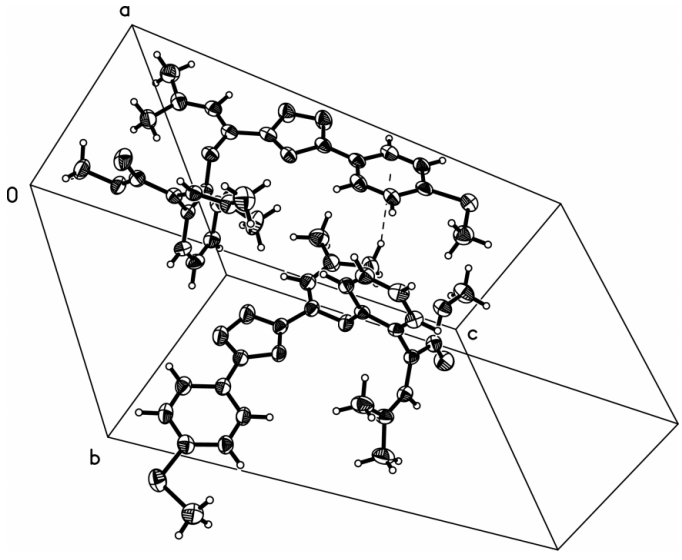


Figure 2
Crystal structure of (I). The dashed line indicates the C—H···π interaction.

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

	D—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20*A*···O3	0.93	2.34	2.756 (5)	107
C23—H23*A*···O1	0.93	2.34	2.757 (3)	107
C25—H25*A*···O2	0.96	2.20	2.959 (5)	135
C25—H25*B*···Cg2^{i}	0.96	2.88	3.783 (1)	158

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$. Cg2 is the centroid of the ring C2—C7.

All H atoms were positioned geometrically at C—H distances of 0.93–0.96 Å and included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq} or 1.5U_{eq} of the carrier atom.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL*97.

References

Enraf–Nonius (1989). *CAD*-4 *Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Harms, K. & Wocadlo, S. (1995). *XCAD*4. University of Marburg, Germany.
Juraszyk, H., Gante, J., Wurziger, H., Bernotat-Danielowski, S. & Melzer, G. (1997). PCT Int. Appl. WO 9744333.
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.
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.