Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

3-[5-(4-Fluorophenyl)-1,3,4-thiadiazol-2-yl]-2-phenylthiazolidin-4-one

Rong Wan,* Feng Wu, Jun Yin and Jin-Tang Wang

Department of Applied Chemistry, College of Science, Nanjing University of Technology, No. 5 Xinmofan Road, Nanjing 210009, People's Republic of China

Correspondence e-mail: rwan01@jlonline.com

Received 6 January 2006
Accepted 19 January 2006
Online 25 January 2006

Key indicators

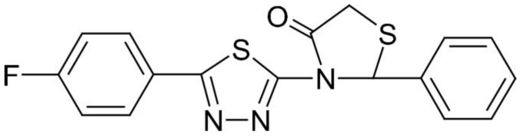
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.047
wR factor = 0.143
Data-to-parameter ratio = 14.0

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

The title compound, $C_{17}H_{12}FN_3OS_2$, was synthesized by the reaction of benzylidene[5-(4-fluorophenyl)-1,3,4-thiadiazol-2-yl]amine and mercaptoacetic acid. The thiazolidinone ring adopts a twist conformation. The thiadiazole ring is a planar aromatic heterocycle.

Comment

Thiadiazole derivatives containing the thiazolidinone unit are of great interest because of their chemical and pharmaceutical properties. Some derivatives have fungicidal activities and exhibit some herbicidal activities (Chen *et al.*, 2000; Kidwai *et al.*, 2000; Vicentini *et al.*, 1998), and some show insecticidal activities (Arun *et al.*, 1999; Wasfy *et al.*, 1996). We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The thiazolidinone ring adopts a twist conformation; the dihedral angle between the C7/C8/S1 and C7/N1/C8 planes is 25.54 (15)°. The thiadiazole ring is a planar aromatic heterocycle. The angle between the thiadiazole and p-fluorobenzene rings is 2.8 (2)°. The phenyl substituent is approximately perpendicular to the mean plane of the thiazolidinone ring because of the lack of conjugation through the saturated sp^3 atom C7.

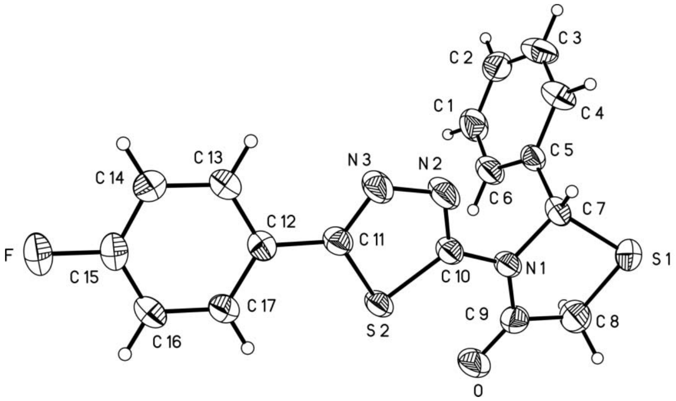


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% level.

Experimental

For the preparation of the title compound, benzylidene[5-(4-fluorophenyl)-1,3,4-thiadiazol-2-yl]amine (5 mmol) and mercaptoacetic acid (5 mmol) were dissolved in toluene (50 ml). The resulting water was removed by distillation over a period of 5 h. The reaction mixture was left to cool to room temperature and filtered, and the resulting solid was recrystallized from acetone to give pure compound (I) (m.p. 513–514 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an acetone solution. ^{1}H NMR ($CDCl_3$, p.p.m.): δ 7.90–7.88 (*m*, 2H), 7.35–7.31 (*m*, 4H), 7.29–7.21 (*m*, 1H), 6.73 (*s*, 1H), 4.16–4.12 (*d*, 1H), 3.89–3.85 (*d*, 1H).

Crystal data

$C_{17}H_{12}FN_3OS_2$
$M_r = 357.42$
Triclinic, $P\bar{1}$
$a = 6.4630$ (13) Å
$b = 10.911$ (2) Å
$c = 11.371$ (2) Å
$\alpha = 97.91$ (3)°
$\beta = 94.37$ (3)°
$\gamma = 99.12$ (3)°
$V = 780.2$ (3) Å^3

$Z = 2$
$D_x = 1.521$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 10$–13°
$\mu = 0.36$ mm^{-1}
$T = 293$ (2) K
Block, colorless
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.869$, $T_{max} = 0.931$
3325 measured reflections
3042 independent reflections
2379 reflections with $I > 2\sigma(I)$

$R_{int} = 0.015$
$\theta_{max} = 26.0$°
$h = 0 \rightarrow 7$
$k = -13 \rightarrow 13$
$l = -13 \rightarrow 13$
3 standard reflections every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.143$
$S = 0.99$
3042 reflections
217 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C8	1.801 (3)	N1—C9	1.374 (3)
S1—C7	1.829 (3)	N1—C10	1.388 (3)
S2—C10	1.728 (2)	N1—C7	1.474 (3)
S2—C11	1.740 (3)	N2—C10	1.297 (3)
F—C15	1.361 (3)	N2—N3	1.381 (3)
O—C9	1.216 (3)	N3—C11	1.295 (3)
C8—S1—C7	91.81 (12)	O—C9—N1	123.1 (2)
C10—S2—C11	85.91 (12)	O—C9—C8	125.4 (3)
C9—N1—C10	123.3 (2)	N1—C9—C8	111.5 (2)
C9—N1—C7	117.4 (2)	N2—C10—N1	120.6 (2)
C10—N1—C7	118.5 (2)	N2—C10—S2	115.50 (19)
C10—N2—N3	111.3 (2)	N1—C10—S2	123.92 (18)
C11—N3—N2	113.2 (2)	N3—C11—C12	123.3 (2)
N1—C7—C5	112.8 (2)	N3—C11—S2	114.04 (19)
N1—C7—S1	103.89 (16)	C12—C11—S2	122.63 (19)
C5—C7—S1	112.24 (17)	F—C15—C16	118.7 (2)
C9—C8—S1	107.2 (2)	F—C15—C14	118.3 (2)

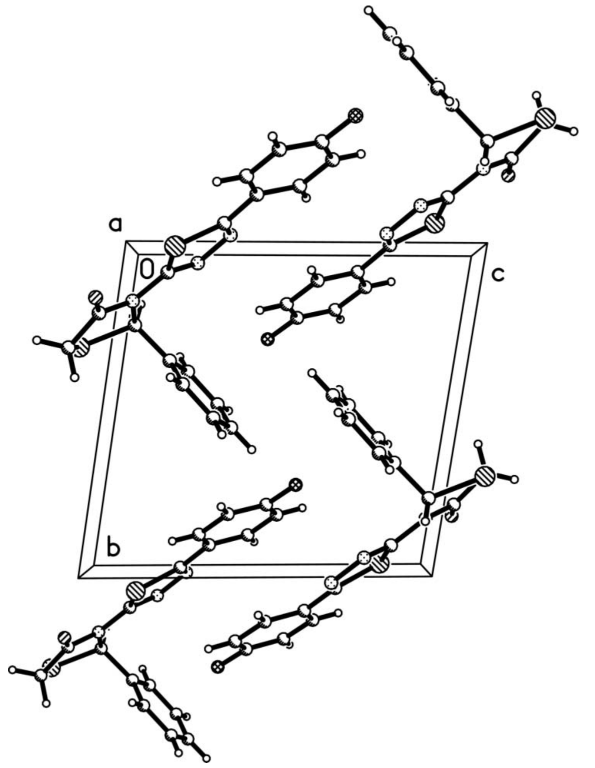


Figure 2
The crystal structure of (I).

All H atoms were positioned geometrically, with C—H distances of 0.93–0.98 Å, and included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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*.

References

Arun, K. P., Nag, V. L. & Panda, C. S. (1999). *Indian J. Chem. Sect. B*, **38**, 998–1001.

Chen, H. S., Li, Z. M. & Han, Y. F. (2000). *J. Agric. Food. Chem.* **48**, 5312–5315.

Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.

Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.

Kidwai, M., Negi, N. & Misra, P. (2000). *J. Indian Chem. Soc.* **77**, 46–48.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

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.

Vicentini, C. B., Manfrini, M., Veronese, A. C. & Guarneri, M. (1998). *J. Heterocycl. Chem.* **35**, 29–36.

Wasfy, A. A., Nassar, S. A. & Eissa, A. M. (1996). *Indian J. Chem. Sect. B*, **35**, 1218–1220.

Acta Cryst. (2006). E**62**, o746–o747 Wan *et al.* • $C_{17}H_{12}FN_3OS_2$ **o747**