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1-(4-Fluorophenyl)-2-(3-phenylthiazolidin-2-ylidene)-2-(1*H*-1,2,4-triazol-1-yl)ethanone

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.073
wR factor = 0.152
Data-to-parameter ratio = 14.4

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

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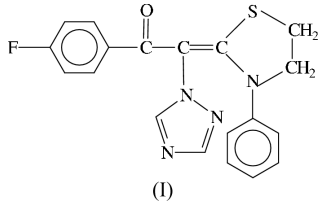
In the title compound, $C_{19}H_{15}FN_4OS$, the dihedral angles between the planes of the triazole and the unsubstituted and F-substituted benzene rings are 23.0 (2) and 65.6 (6)°, respectively, while that between the two benzene rings is 87.4 (0)°. There are some intermolecular and intramolecular interactions in the crystal structure.

Comment

An important type of fungicides, triazole compounds are highly efficient and have low toxicity (Shi *et al.*, 1995; Xu *et al.*, 2002). At present, studies on triazole derivatives are mainly concentrated on compounds with triazole as the only active group. There are few reports of triazole compounds that contain both a triazole group and another active group in a single molecule. Considering that triazole compounds have different fungicidal mechanisms than thiazole compounds, it is possible that the two kinds of *N*-heterocyclic groups increase the fungicidal activity and fungicidal spectrum. In the search for new triazole and thiazole compounds with higher bioactivity, the title compound, (I), was synthesized.



(I)

In the title compound, the bond lengths and angles in the 1,2,4-triazole ring and two benzene rings are normal (Ji *et al.*, 2002). The bond lengths and angles in the thiazolidine ring are also in good agreement with those reported previously (Domagała *et al.*, 2003). The C—F bond length [1.354 (4) Å] is similar to those found by Lynch & McClenaghan (2004) [1.340 (3)–1.345(3 Å)]. The C9—C10 bond length of 1.377 (4) Å is indicative of considerable double-bond character.

The seven atoms S1, N1, N2, C7, C9, C10 and C13 are coplanar (*p*1). The dihedral angles formed by *p*1 and the benzene rings C1–C6 (*p*2) and C14–C19 (*p*3), and the triazole ring (*p*4) are 68.2 (2), 59.9 (5) and 63.9 (1)°, respectively. The dihedral angles formed by *p*2 and *p*3 with *p*4 are 23.0 (2) and 65.6 (6)°, respectively. The dihedral angle between *p*2 and *p*3 is 87.4 (0)°.

The Cremer & Pople (1975) puckering amplitude of the thiazolidine ring is q_2 = 0.0.264(5) Å. According to Duax *et al.* (1976), the conformation is an envelope with a local pseudo-

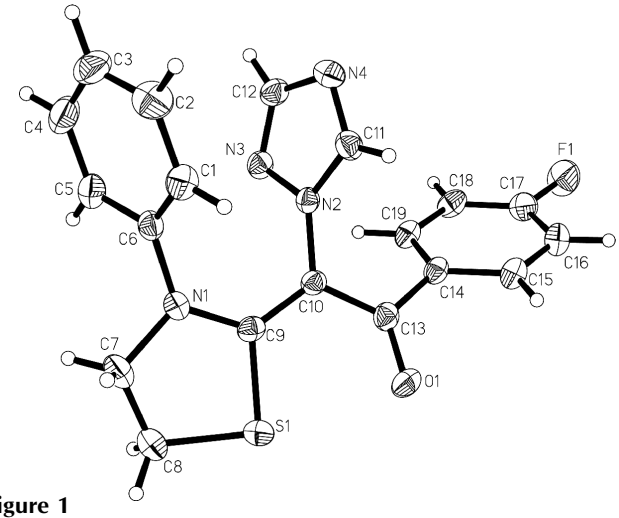


Figure 1
The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

mirror passing through C8 and the mid-point of the N1—C9 bond.

There are some weak C—H···*Y* (*Y* = F, O and N) intermolecular interactions (see Table 2) which stabilize the title structure.

Experimental

The title compound was prepared by reaction of [α-(1,2,4-triazol-1-yl)]-4-fluoroacetophenone (0.02 mmol), phenyl isothiocynate (0.02 mmol) and $BrCH_2CH_2Br$ (0.02 mmol) in DMSO solution (40 ml). Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization from chloroform/ethyl acetate (*v*/*v* = 1:3) at room temperature.

Crystal data

$C_{19}H_{15}FN_4OS$
M_r = 366.41
Triclinic, $P\overline{1}$
a = 9.3895 (19) Å
b = 9.6613 (19) Å
c = 10.929 (2) Å
α = 111.53 (3)°
β = 100.46 (3)°
γ = 102.08 (3)°
V = 864.7 (4) Å^3
Z = 2
D_x = 1.407 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
θ = 2–11°
μ = 0.21 mm^{-1}
T = 293 (2) K
Block, yellow
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: none
3976 measured reflections
3382 independent reflections
2441 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.9°
$h = -6 \rightarrow 11$
$k = -12 \rightarrow 11$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.152
S = 1.11
3382 reflections
235 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected torsion angles (°).

C6—N1—C9—C10	−14.9 (5)	N1—C9—C10—N2	−0.1 (5)
C7—N1—C9—S1	−0.3 (4)	S1—C9—C10—N2	177.5 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*A*···N4^{i}	0.93	2.61	3.519 (6)	168
C4—H4*B*···F1^{ii}	0.93	2.53	3.317 (5)	143
C11—H11*A*···O1^{iii}	0.93	2.38	3.279 (7)	164

Symmetry codes: (i) $1-x, 2-y, -z$; (ii) $x-1, y, z-1$; (iii) $1-x, 2-y, 1-z$.

The H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, with $U_{iso} = 1.2U_{eq}$(parent atom).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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References

Duax, W. L., Weeks, C. M. & Roher, D. C. (1976). *Topics in Stereochemistry*, Vol. 9, edited by E. L. Eliel & N. Allinger, pp. 271–383. New York: John Wiley.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Domagała, M., Linden, A., Olszak, T. A., Mloston, G. & Heimgartner, H. (2003). *Acta Cryst.* C**59**, o250–o253.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Ji, B. M., Du, C. X., Zhu, Y. & Wang, Y. (2002). *Chin. J. Struct. Chem.* **21**, 252–255.
Lynch, D. E. & McClenaghan, L. (2004). *Acta Cryst.* C**60**, o1–o5.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1990). *SHELXTL/PC Users' Manual.* Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-Ray Systems Inc., Madison, Wisconsin, USA.
Shi, Y. N., Lu, Y. C. & Fang, J. X. (1995). *Chem. J. Chin. Univ.*, **16**, 1710–1713.
Xu, L. Z., Zhang, S. S., Li, H. J. & Jiao, K. (2002). *Chem. Res. Chin. Univ.* **18**, 284–286.