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3-Anilino-1-(2-fluoro-5-methylphenyl)-3-(methylsulfanyl)-2-(1*H*-1,2,4-triazol-1-yl)prop-2-en-1-one

Liangzhong Xu,* Chongyi Zhu, Guodong Si, Yongqi Qin and Kai Li

Institute of Agricultural Chemicals, Qingdao University of Science and Technology, Qingdao, 266042, People's Republic of China

Correspondence e-mail: qknhs@163169.net

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.125
Data-to-parameter ratio = 15.9

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

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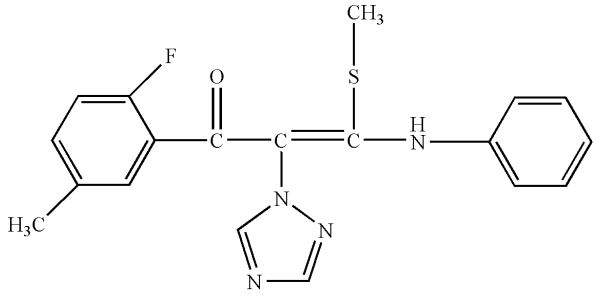
The title compound, $C_{19}H_{17}FN_4OS$, was synthesized by reacting (2-fluoro-5-methyl)-1*H*-(1,2,4-triazol-1-yl)acetophenone with phenyl isothiocyanate and methyl iodide in an ethanol solution. Intermolecular and intramolecular hydrogen-bond interactions stabilize the structure.

Comment

Recently, compounds containing a 1*H*-1,2,4-triazole group have attracted much interest because compounds containing a triazole ring system are well known as efficient fungicides in pesticides and medicine by inhibiting the biosynthesis of ergosterol, and have good plant-growth regulatory activity for a wide variety of crops (Xu *et al.*, 2002). In order to search for new triazole compounds with higher bioactivity, we have synthesized the title compound, (I), and describe its structure here.



(I)

In the title compound, bond lengths and angles are as expected. The group of atoms C9, C8, O1 and C7 is planar (plane *p*1). The six atoms S1,N1,N4,C8,C9,C12 lie in a plane (*p*2). The dihedral angles formed by the benzene rings [C2,C3,C4,C5,C6,C7], [C14,C15,C16,C17,C18,C19] and the triazole ring with *p*1 and *p*2 are 47.8 (3), 44.2 (4) and 77.8 (5), and 51.6 (5), 44.7 (1) and 74.5 (3)°, respectively. The dihedral angle between *p*1 and *p*2 is 6.1 (2)°.

The intramolecular and intermolecular hydrogen-bond interactions (Table 2), which stabilize the structure, are the most interesting structural feature of the title compound.

Experimental

The title compound was prepared by reaction of (2-fluoro-5-methyl)-1*H*-(1,2,4-triazol-1-yl)acetophenone (4.14 g, 0.02 mol), phenyl isothiocyanate (2.24 g, 0.02 mol), potassium hydroxide (2.24 g, 0.04 mol) and methyl iodide (2.83 g, 0.02 mol) in 30 ml ethanol solution at room temperature. Single crystals of the title compound, suitable for X-ray analysis, were obtained by recrystallization from chloroform/ethyl acetate (*v*/*v* = 1:3) at room temperature.

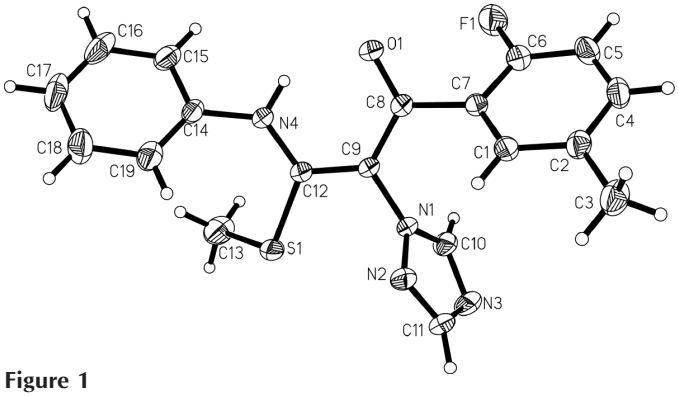


Figure 1
The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Crystal data

$C_{19}H_{17}FN_4OS$	D_x = 1.329 Mg m^{-3}
M_r = 368.43	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 905 reflections
a = 19.651 (6) Å	θ = 2.4–26.3°
b = 5.6123 (11) Å	μ = 0.20 mm^{-1}
c = 17.187 (3) Å	T = 293 (2) K
β = 103.76 (3)°	Block, yellow
V = 1841.1 (8) Å^3	0.30 × 0.20 × 0.18 mm
Z = 4	

Data collection

Bruker SMART CCD area detector diffractometer	2690 reflections with $I > 2\sigma(I)$
	R_{int} = 0.027
φ and ω scans	θ_{max} = 26.4°
Absorption correction: none	$h = -24 \rightarrow 23$
10219 measured reflections	$k = -7 \rightarrow 6$
3755 independent reflections	$l = -21 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0643P)^2 + 0.551P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.042	
$wR(F^2)$ = 0.125	
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
3755 reflections	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
236 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

S1—C12	1.7614 (19)	O1—C8	1.246 (2)
S1—C13	1.793 (3)	N4—C12	1.342 (2)
F1—C6	1.354 (2)		
C12—S1—C13	103.44 (11)	C12—N4—H4	114.6
C12—N4—C14	130.85 (17)	C7—C1—C2	122.23 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O1	0.86	1.93	2.606 (2)	135
C10—H10···N2^{i}	0.93	2.61	3.444 (3)	150
C11—H11···N3^{ii}	0.93	2.53	3.433 (3)	164
C19—H19···S1	0.93	2.84	3.275 (3)	110

Symmetry codes: (i) $x, y-1, z$; (ii) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$.

The H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding, with U_{iso}(H) = 1.2 and 1.5 times U_{eq} of the parent atoms.

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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