

## 2-Fluoro-5-methylphenyl (1*H*-1,2,4-triazol-1-yl)-(1,1,3-trioxo-1,2-dihydro-1,2-benzothiazol-2-yl)-methyl ketone

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### Key indicators

Single-crystal X-ray study

$T = 294\text{ K}$

Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$

$R$  factor = 0.056

$wR$  factor = 0.117

Data-to-parameter ratio = 14.2

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

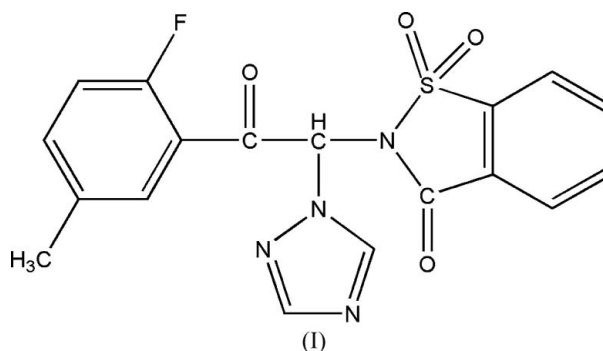
In the title compound,  $\text{C}_{18}\text{H}_{13}\text{FN}_4\text{O}_4\text{S}$ , the dihedral angles between the planes of the triazole and the sulfobenzimidazole ring and benzene ring are  $87.69(3)$  and  $74.35(2)^\circ$ , respectively. There are weak intermolecular hydrogen-bond interactions that assemble the molecules into slabs parallel to the  $bc$  plane.

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### Comment

As an important type of fungicide, triazole compounds are highly efficient and of low toxicity (Shi *et al.*, 1995; Xu *et al.*, 2002). On the other hand, sulfobenzimidazole is used for diuretic (Chien, 1959), ataratic (Vnederlands, 1965) and soporific applications (Graadums *et al.*, 1973), and some compounds containing the sulfobenzimidazole group possess highly fungicidal and phytocidal activity (Hlasta *et al.*, 1993; Hanagan & Pasteris, 1986). Thus, since triazole compounds have a different fungicidal mechanism from that of sulfobenzimidazole compounds, it was expected that a compound with both groups, such as title compound, (I) (Fig. 1), would have an enhanced fungicidal activity.



In (I), the C9–N4 and C10–N3 bond lengths (Table 1) are close to the typical C=N double-bond length [ $1.330(3)\text{ \AA}$ ; Dean, 1998], which reveals that these two bonds have features of unsaturated double bonds. The dihedral angles between the planes of the triazole and the sulfobenzimidazole ring and benzene ring are  $87.69(3)$  and  $74.35(2)^\circ$ , respectively. There are some weak C–H...O and C–H...F intermolecular hydrogen bonds in the crystal structure, assembling the molecules into slabs parallel to the  $bc$  plane (Fig. 2, Table 2).

### Experimental

Triethylamine (0.022 mol) was dissolved in acetone (5 ml) and a mixture of 2-fluoro-2-(1*H*-1,2,4-triazole-1-yl)acetophenone (0.02 mol), sulfobenzimidazole (0.02 mol) and acetone (20 ml) was

added dropwise with stirring at 273 K for 2 h, and then for 10 h at room temperature. The solution was then filtered, concentrated and purified by chromatography on a silica gel column to give a white solid (yield 34%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol and ethyl acetate (1:2) at room temperature.

Crystal data

$C_{18}H_{13}FN_4O_4S$   
 $M_r = 400.38$   
 Monoclinic,  $C2/c$   
 $a = 21.269 (5) \text{ \AA}$   
 $b = 10.594 (3) \text{ \AA}$   
 $c = 15.758 (4) \text{ \AA}$   
 $\beta = 94.823 (4)^\circ$   
 $V = 3538.0 (15) \text{ \AA}^3$

$Z = 8$   
 $D_x = 1.503 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.23 \text{ mm}^{-1}$   
 $T = 294 (2) \text{ K}$   
 Block, white  
 $0.22 \times 0.14 \times 0.06 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.952, T_{\max} = 0.987$

9516 measured reflections  
 3609 independent reflections  
 2137 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.060$   
 $\theta_{\text{max}} = 26.4^\circ$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.056$   
 $wR(F^2) = 0.117$   
 $S = 1.07$   
 3609 reflections  
 254 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0309P)^2 + 4.2871P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.37 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.46 \text{ e \AA}^{-3}$

Table 1

Selected bond lengths (Å).

F1—C13	1.358 (4)	N4—C9	1.312 (4)
N3—C10	1.322 (4)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C5—H5...O4 <sup>i</sup>	0.93	2.54	3.464 (4)	173
C8—H8...O1 <sup>ii</sup>	0.98	2.27	3.000 (4)	130
C10—H10...O3 <sup>iii</sup>	0.93	2.45	3.375 (4)	175
C14—H14...F1 <sup>iv</sup>	0.93	2.49	3.394 (4)	163

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

All H atoms were placed in calculated positions, with C—H = 0.93–0.98 Å, and refined using a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ , or  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl H atoms.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

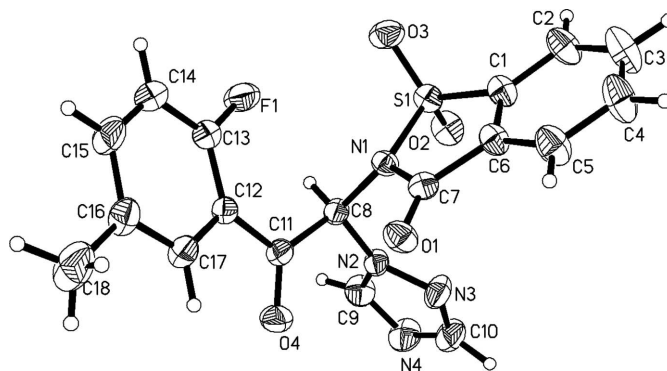


Figure 1 The molecular structure of (I), with displacement ellipsoids drawn at the 40% probability level.

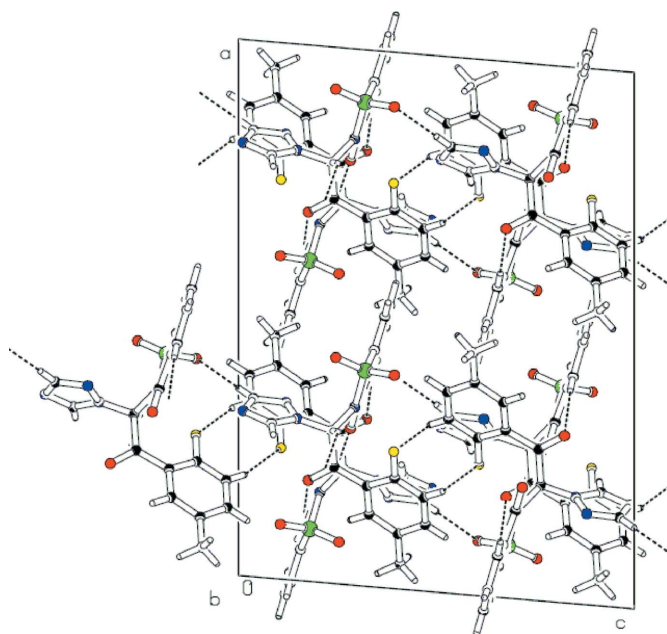


Figure 2 A packing diagram of the title compound; viewed down the  $b$  axis. Hydrogen bonds are shown as dashed lines.

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