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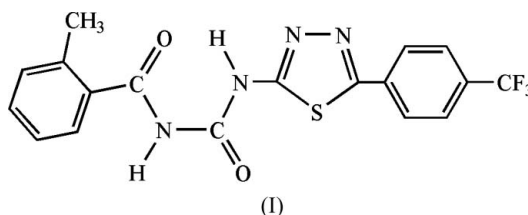
Key indicators

Single-crystal X-ray study
T = 292 K
Mean $\sigma(C-C)$ = 0.004 Å
Disorder in main residue
R factor = 0.049
wR factor = 0.148
Data-to-parameter ratio = 11.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

1-(2-Methylbenzoyl)-3-{5-[4-(trifluoromethyl)-phenyl]-1,3,4-thiadiazol-2-yl}urea

In the title compound, C₁₈H₁₃F₃N₄O₂S, the urea linkage is essentially planar due to the presence of an intramolecular N—H···O hydrogen bond. Intermolecular N—H···O hydrogen bonds link two neighbouring molecules into a centrosymmetric *R*₂²(8) dimer.

Comment

1,3,4-Thiadiazole derivatives represent an interesting class of compounds possessing broad-spectrum biological properties (Foroumadi *et al.*, 2002; Wang, Wang *et al.*, 2004). Aroyl ureas are known to exhibit diverse biological effects, such as insecticidal, fungicidal, herbicidal and plant-growth-regulating activities (Chen *et al.*, 2005; Wang *et al.*, 1998). Considerable interest has been shown in fluorine-containing compounds. It is therefore worth investigating fluoro derivatives incorporating both a 1,3,4-thiadiazole nucleus and an aroyl urea group. In a previous paper (Wang, Zhao *et al.*, 2004), a series of aroyl ureas containing a 1,3,4-thiadiazole ring have been reported to have good activity as plant-growth regulators. In view of this and as a continuation of our research on the biological properties of this class, a number of new compounds have been synthesized in our laboratory, including the title compound, (I).The crystal structure (Fig.1) reveals that the urea linkage unit O2—C11—N4—C10—N3—H3A adopts the most stable conformation for the formation of an intramolecular N—H···O hydrogen bond (Song *et al.*, 2005), giving a planar six-membered ring. Selected bond lengths and angles are listed in Table 1. In the crystal structure, the molecules are linked by pairs of N—H···O hydrogen bonds into centrosymmetric *R*₂²(8) dimers (Bernstein *et al.*, 1995; Glidewell *et al.*, 2003) (Fig. 2 and Table 2).

Experimental

The title compound (I) was prepared according to the procedure of Wang *et al.* (2003). Suitable crystals were obtained by vapor diffusion of methanol into a DMF solution at room temperature (m.p. >573 K). Elemental analysis: analysis calculated for C₁₈H₁₃F₃N₄O₂S: C 53.20, H 3.22, N 13.79%; found: C 53.11, H 3.35, N 13.62%.

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Crystal data

$C_{18}H_{13}F_3N_4O_2S$
 $M_r = 406.38$
 Monoclinic, $P2_1/c$
 $a = 16.844$ (2) Å
 $b = 7.3080$ (11) Å
 $c = 15.202$ (2) Å
 $\beta = 104.964$ (2)°
 $V = 1807.9$ (4) Å³
 $Z = 4$

$D_x = 1.493$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 2599 reflections
 $\theta = 2.5$ – 24.0 °
 $\mu = 0.23$ mm⁻¹
 $T = 292$ (2) K
 Block, colorless
 $0.30 \times 0.20 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: none
 8650 measured reflections
 3169 independent reflections

2619 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.028$
 $\theta_{max} = 25.0$ °
 $h = -19 \rightarrow 20$
 $k = -8 \rightarrow 7$
 $l = -16 \rightarrow 18$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.148$
 $S = 1.10$
 3169 reflections
 282 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0849P)^2 + 0.1744P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.31$ e Å⁻³
 $\Delta\rho_{min} = -0.37$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

C1–C2	1.491 (5)	C10–O1	1.217 (3)
C5–C8	1.469 (3)	C10–N3	1.348 (3)
C8–N1	1.291 (3)	C10–N4	1.388 (3)
C8–S1	1.733 (2)	C11–O2	1.222 (3)
C9–N2	1.295 (3)	C11–N4	1.376 (3)
C9–N3	1.381 (3)	C11–C12	1.490 (4)
C9–S1	1.718 (2)	C13–C18	1.502 (4)
C3–C2–C1	120.1 (3)	N3–C10–N4	116.3 (2)
C7–C2–C1	120.1 (3)	O2–C11–N4	121.7 (2)
C6–C5–C8	119.5 (2)	O2–C11–C12	123.5 (2)
N1–C8–C5	122.7 (2)	N4–C11–C12	114.8 (2)
N1–C8–S1	114.08 (19)	C12–C13–C18	123.4 (2)
C5–C8–S1	123.24 (19)	C8–N1–N2	113.0 (2)
N2–C9–N3	120.2 (2)	C9–N2–N1	111.5 (2)
N2–C9–S1	115.26 (19)	C10–N3–C9	123.0 (2)
N3–C9–S1	124.57 (18)	C11–N4–C10	127.8 (2)
O1–C10–N3	122.8 (2)	C9–S1–C8	86.18 (12)
O1–C10–N4	121.0 (2)		
C1–C2–C3–C4	179.7 (3)	N3–C9–N2–N1	177.7 (2)
C1–C2–C7–C6	–179.9 (3)	S1–C9–N2–N1	–0.8 (3)
C6–C5–C8–N1	–31.0 (4)	C8–N1–N2–C9	–0.3 (3)
C4–C5–C8–N1	147.6 (3)	O1–C10–N3–C9	6.2 (4)
C6–C5–C8–S1	148.5 (2)	N4–C10–N3–C9	–174.3 (2)
C4–C5–C8–S1	–32.9 (4)	N2–C9–N3–C10	166.6 (2)
O2–C11–C12–C17	–142.1 (3)	S1–C9–N3–C10	–15.0 (3)
N4–C11–C12–C17	36.8 (3)	O2–C11–N4–C10	–5.3 (4)
O2–C11–C12–C13	35.7 (4)	C12–C11–N4–C10	175.8 (2)
N4–C11–C12–C13	–145.4 (2)	O1–C10–N4–C11	–174.3 (2)
C17–C12–C13–C14	1.4 (4)	N3–C10–N4–C11	6.1 (4)
C11–C12–C13–C14	–176.4 (2)	N2–C9–S1–C8	1.2 (2)
C17–C12–C13–C18	–174.5 (3)	N3–C9–S1–C8	–177.2 (2)
C11–C12–C13–C18	7.7 (4)	N1–C8–S1–C9	–1.4 (2)
C5–C8–N1–N2	–179.2 (2)	C5–C8–S1–C9	179.1 (2)
S1–C8–N1–N2	1.3 (3)		

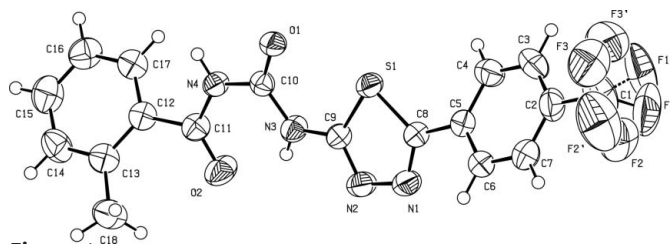


Figure 1

View of the molecule of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size. Both disorder components are shown.

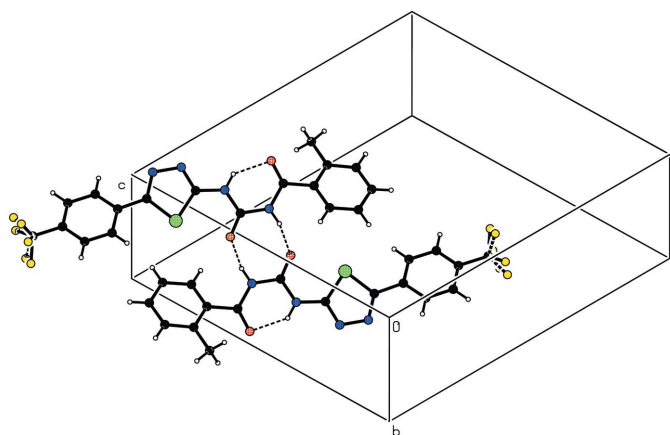


Figure 2

A partial packing diagram of (I), showing the hydrogen bonding (dashed lines).

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N3-H3A\cdots O2$	0.86	1.95	2.614 (3)	133
$N4-H4A\cdots O1^i$	0.86	2.13	2.853 (3)	141

Symmetry code: (i) $-x, -y, -z + 1$.

All H atoms were initially located in a difference Fourier map. Methyl H atoms were then constrained to an ideal geometry with C–H distances of 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$, but each group was allowed to rotate freely about its C–C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H distances of 0.93 Å, N–H distances of 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The occupancies of the disordered positions F/F' were refined to 0.432 (16)/0.568 (16).

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Sheldrick, 2001); software used to prepare material for publication: SHELXTL.

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