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## Key indicators

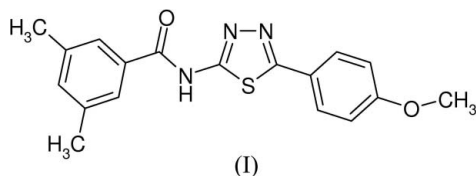
Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
 $R$  factor = 0.052  
 $wR$  factor = 0.162  
Data-to-parameter ratio = 14.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.***N*-[5-(4-Methoxyphenyl)-1,3,4-thiadiazol-2-yl]-3,5-dimethylbenzamide**

The title compound,  $\text{C}_{18}\text{H}_{17}\text{N}_3\text{O}_2\text{S}$ , was synthesized by reaction of [5-(4-methoxyphenyl)-1,3,4-thiadiazol-2-yl]amine with 3,5-dimethylbenzoic acid. In the crystal structure, intermolecular  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds link the molecules into centrosymmetric dimers.

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## Comment

Thiadiazole derivatives containing the benzamide unit are of interest because of their chemical and pharmaceutical properties. Some derivatives have fungicidal properties, exhibiting herbicidal (Chen *et al.*, 2000; Kidwai *et al.*, 2000; Vicentini *et al.*, 1998) or insecticidal activity (Arun *et al.*, 1999; Wasfy *et al.*, 1996).



The molecular structure of (I) is shown in Fig. 1. In the crystal structure, molecules are linked into centrosymmetric dimers through  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds (Table 1 and Fig. 2).

## Experimental

A solution of [5-(4-methoxyphenyl)-1,3,4-thiadiazol-2-yl]amine (5 mmol) in pyridine (50 ml) was cooled to 273 K and 3,5-dimethylbenzoic acid (5 mmol) was added dropwise over a period of 30 min. The mixture was stirred at 273 K for 1 h, then warmed to room temperature and stirred for a further 1 h. The pyridine was then

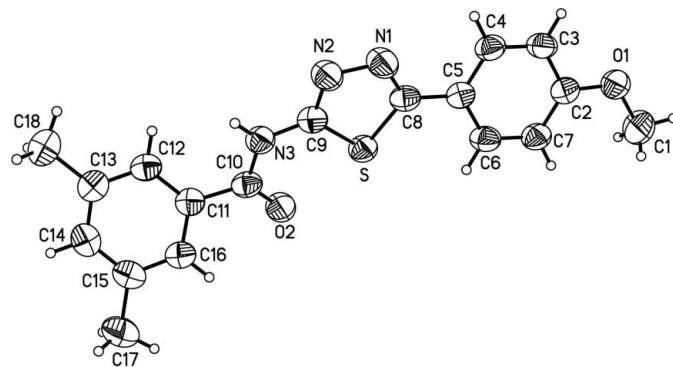


Figure 1

The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level for non-H atoms.

removed by evaporation and the solid was recrystallized from ethanol to provide compound (I) (yield 81%; m.p. 520–524 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an acetone solution.

#### Crystal data

$C_{18}H_{17}N_3O_2S$	$V = 835.9 (3) \text{ \AA}^3$
$M_r = 339.41$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.349 \text{ Mg m}^{-3}$
$a = 7.7105 (14) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.3328 (18) \text{ \AA}$	$\mu = 0.21 \text{ mm}^{-1}$
$c = 14.454 (2) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\alpha = 74.44 (3)^\circ$	Block, colourless
$\beta = 83.07 (3)^\circ$	$0.30 \times 0.10 \times 0.10 \text{ mm}$
$\gamma = 69.18 (3)^\circ$	

#### Data collection

Enraf–Nonius CAD-4 diffractometer	3215 independent reflections
$\omega/2\theta$ scans	2297 reflections with $I > 2\sigma(I)$
Absorption correction: $\psi$ scan (North <i>et al.</i> , 1968)	$R_{\text{int}} = 0.022$
$T_{\text{min}} = 0.940$ , $T_{\text{max}} = 0.979$	$\theta_{\text{max}} = 26.0^\circ$
3460 measured reflections	3 standard reflections every 200 reflections
	intensity decay: none

#### Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.052$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$
$wR(F^2) = 0.162$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\text{max}} < 0.001$
3215 reflections	$\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
217 parameters	$\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$

**Table 1**

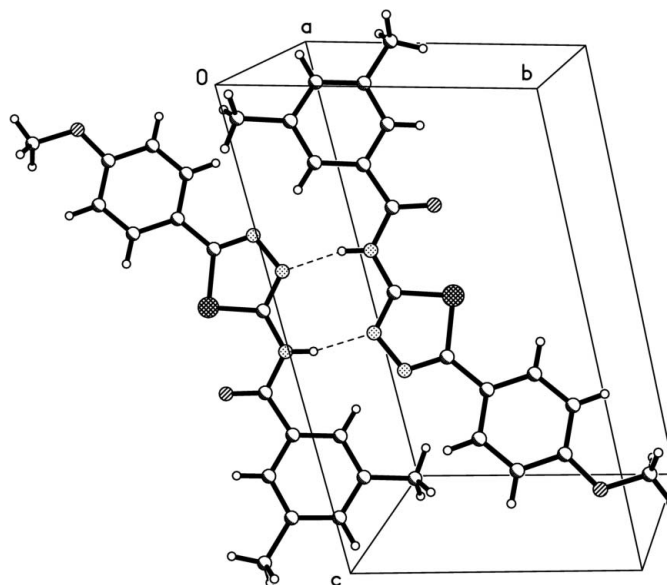
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N3-H3A\cdots N2^i$	0.86	2.18	2.996 (3)	158

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

All H atoms were placed geometrically, with  $C-H = 0.93\text{--}0.97 \text{ \AA}$  and  $N-H = 0.86 \text{ \AA}$ , and allowed to ride during subsequent refinement, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ .

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*



**Figure 2**

The centrosymmetric dimer in (I), linked by  $N-H\cdots N$  hydrogen bonds (dashed lines).

(Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

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