Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3,5-Dimethyl-*N*-(5-*m*-tolyl-1,3,4-thiadiazol-2-yl)-benzamide

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Received 14 January 2007
Accepted 18 January 2007

The title compound, $C_{18}H_{17}N_3OS$, was synthesized by the reaction of 5-*m*-tolyl-1,3,4-thiadiazol-2-amine and 3,5-dimethylbenzoyl chloride. Molecules of the compound are linked by intermolecular N—H···N hydrogen bonds to form centrosymmetric dimers.

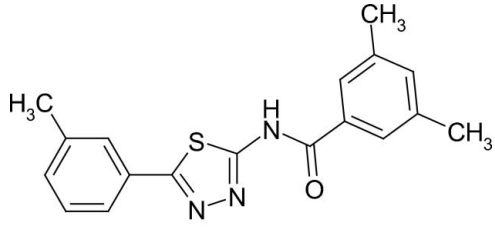
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.137
Data-to-parameter ratio = 15.0

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

Comment

1,3,4-Thiadiazole derivatives represent an interesting class of compounds possessing a broad spectrum of biological activities (Nakagawa *et al.*, 1996; Wang *et al.*, 1999). These compounds are known to exhibit diverse biological effects, such as insecticidal and fungicidal activities (Wang *et al.*, 1999). We present here the crystal structure of the title 1,3,4-thiadiazole derivative, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The thiadiazole ring forms dihedral angles of 14.1 (2)° with the methylphenyl ring and 16.8 (1)° with the dimethylphenyl ring.

N—H···N hydrogen bonds link the molecules to form centrosymmetric dimers (Fig. 2 and Table 1).

Experimental

For the preparation of the title compound, a solution of 5-*m*-tolyl-1,3,4-thiadiazol-2-amine (5 mmol) in pyridine (50 ml) was cooled to 273 K. To this solution, 3,5-dimethylbenzoyl chloride (5 mmol) was added *via* a dropping funnel over a period of 30 min. The mixture was stirred at 273 K for 1 h, warmed to room temperature and reacted for 1 h. The pyridine was distilled off and the resulting solid was recrystallized from ethanol (m.p. 520–524 K). Crystals of (I) were obtained by slow evaporation of an acetone solution.

Crystal data

$C_{18}H_{17}N_3OS$
M_r = 323.41
Triclinic, $P\overline{1}$
a = 8.6420 (17) Å
b = 9.0980 (18) Å
c = 10.924 (2) Å
α = 84.08 (3)°
β = 72.59 (3)°
γ = 79.42 (3)°
V = 804.6 (3) Å^3
Z = 2
D_x = 1.335 Mg m^{-3}
Mo *Kα* radiation
μ = 0.21 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

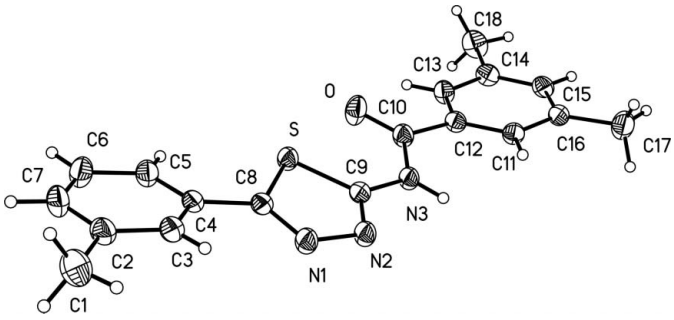


Figure 1
A view of the molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

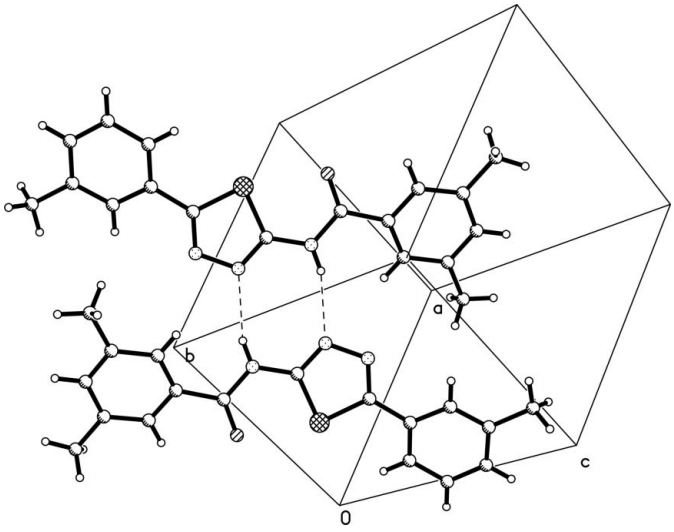


Figure 2
A packing view of (I), showing the hydrogen bonds as dashed lines.

Data collection

Enraf–Nonius CAD4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.940, T_{max} = 0.979
3157 measured reflections
3157 independent reflections
2482 reflections with $I > 2\sigma(I)$
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.137
S = 1.05
3157 reflections
211 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 0.18P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N2^{i}	0.86	2.21	3.036 (3)	160

Symmetry code: (i) $-x+2, -y+2, -z+1$.

All H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and were included in the refinement in a riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}). The methyl groups were allowed to rotate but not to tip.

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

The authors gratefully acknowledge Professor Hua-Qin Wang of the Analysis Centre, Nanjing University, for providing the Enraf–Nonius CAD4 diffractometer for this research project.

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