# N-(4,6-Dimethyl-2,3-dihydropyrimidin-2-ylidene)benzenesulfonamide

**Gong-Chun Li\* and Feng-Ling Yang**

Department of Chemistry, Xuchang University, Xuchang Henan Province 461000, People's Republic of China

Correspondence e-mail:
ligongchun@yahoo.com.cn

**Key indicators**

Single-crystal X-ray study

$T$ = 294 K

Mean $\sigma$(C–C) = 0.003 Å

$R$ factor = 0.035

$wR$ factor = 0.100

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.

In the crystal structure of the title compound, $C_{12}H_{13}N_3O_2S$, weak intermolecular C—H···O and N—H···O hydrogen-bond interactions link the molecules into a double chain along the $b$ axis. In the title molecule, the plane of the pyrimidine ring makes an angle of 87.51 (5)° with the plane of the phenyl ring.

## Comment

Pyrimidine derivatives are very important molecules in biology and have many applications in the areas of pesticides and pharmaceutical agents (Condon *et al.*, 1993). For example, imazosulfuron, ethirmol and mepanipyrim have been commercialized as agrochemicals (Maeno *et al.*, 1990). Pyrimidine derivatives have also been developed as antiviral agents, such as AZT (azidothymidine), which is the most widely used anti-AIDS drug (Gilchrist, 1997). In a quest for further biologically active pyrimidine compounds, the title compound, (I), has been synthesized and its crystal structure determined (Fig. 1).



(I)
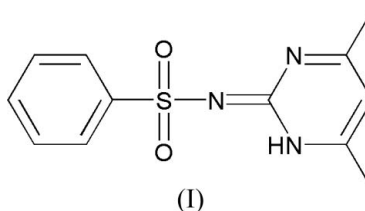
In (I), the heterocycle contains the structural unit N2—C—N3H rather than N2—C=N3, an H atom being transferred from N1 to N3; it makes an angle of 87.51 (5)° with the plane of the phenyl ring. In the crystal structure, there are intermolecular C—H···O and N—H···O hydrogen-bond interactions which link the molecules into a double chain along the $b$-axis direction (Fig. 2).

## Experimental

Benzenesulfonyl chloride (0.37 g, 2.1 mmol) was added to a mixture of anhydrous pyridine (4 ml) and 4,6-dimethylpyrimidin-2-amine (0.25 g, 2 mmol). The mixture was heated slowly to 333 K, and then maintained at that temperature for 5 h. The solvent was evaporated *in vacuo* and water (5 ml) was added to the residue. The resulting brown precipitate was filtered off, dissolved in ethanol (10 ml) and decolourized with active carbon, giving the title compound, (I) (0.27 g, 52% yield). The title compound was recrystallized from ethanol giving single crystals (m.p. 419–420 K).
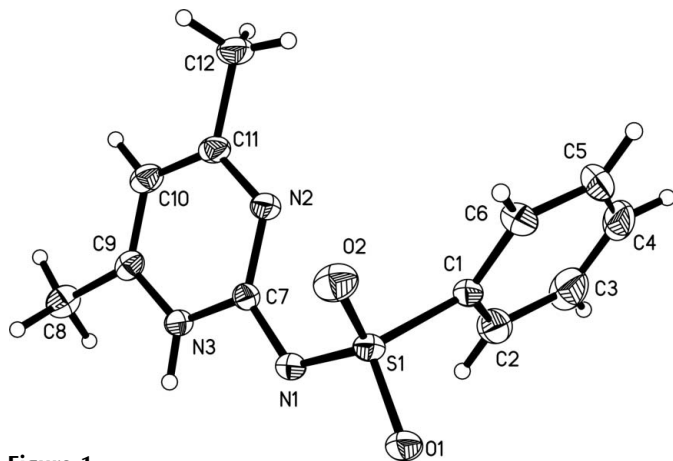
**Figure 1**
The asymmetric unit of the title compound, (I), with displacement ellipsoids drawn at the 30% probability level.

*Crystal data*

$C_{12}H_{13}N_3O_2S$
$M_r = 263.31$
Monoclinic, $P2_1/c$
$a = 8.6895 (10)$ Å
$b = 9.0539 (11)$ Å
$c = 15.9006 (18)$ Å
$\beta = 90.888 (2)°$
$V = 1250.8 (3)$ Å$^3$

$Z = 4$
$D_x = 1.398$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu = 0.26$ mm$^{-1}$
$T = 294 (2)$ K
Prism, colourless
$0.24 \times 0.20 \times 0.18$ mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.928$, $T_{max} = 0.955$

6849 measured reflections
2557 independent reflections
2217 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 26.4°$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.100$
$S = 1.07$
2557 reflections
170 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.4241P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å$^{-3}$
$\Delta\rho_{min} = -0.33$ e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.096 (5)

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D \cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| N3—H3$A\cdots$O1$^i$ | 0.91 (2) | 1.91 (2) | 2.8130 (17) | 170.7 (18) |
| C8—H8$B\cdots$O2$^{ii}$ | 0.96 | 2.56 | 3.289 (2) | 133 |

Symmetry codes: (i) $-x + 2, y + \frac{1}{2}, -z + \frac{3}{2}$; (ii) $x, y + 1, z$.

The H atom on N3 was found in a difference Fourier map and refined freely. H atoms bound to C atoms were placed ain calculated
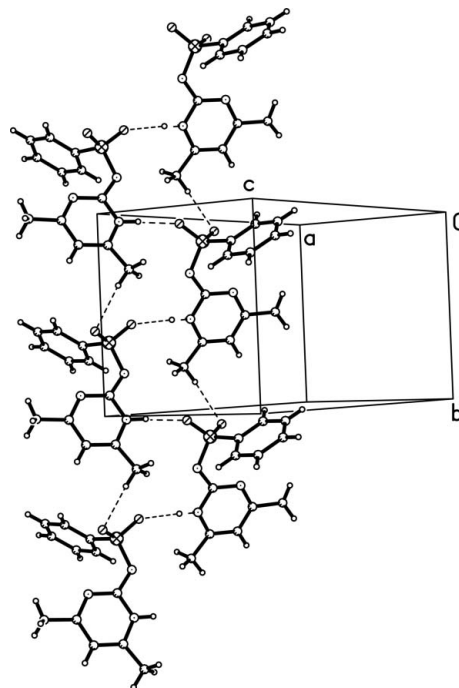


**Figure 2**
A view of the intermolecular C—H$\cdots$O and N—H$\cdots$O hydrogen-bond interactions (dashed lines) in (I).

positions, with C—H = 0.93 or 0.96 Å, and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}$(aromatic C) or $1.5U_{eq}$(methyl C).

Data collection: *SMART* (Bruker, 1999); 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*.

## References

Bruker (1999). *SMART* (Version 5.618), *SAINT* (Version 6.45) and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Condon, M. E., Brady, T. E., Feist, D., Malefyt, T., Marc, P., Quakenbush, L. S., Rodaway, S. J., Shaner, D. L. & Tecle, B. (1993). *Brighton Crop Prot. Conf. Weeds*, pp. 41–46. Alton, Hampshire, England: BCPC Publications.
Gilchrist, T. L. (1997). *Heterocyclic Chemistry*, 3rd ed., pp. 261–276. Singapore: Addison Wesley Longman.
Maeno, S., Miura, I., Masuda, K. & Nagata, T. (1990). *Brighton Crop Prot. Conf. Pests and Diseases*, pp. 415–422. Alton, Hampshire, England: BCPC Publications.
Sheldrick, G. M. (1996). *SADABS*. Version 4.202. University of Göttingen,. Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.