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# 1-(4,6-Dimethylpyrimidin-2-ylsulfanyl)-3,3-dimethylbutan-2-one

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**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
*R* factor = 0.044
*wR* factor = 0.122
Data-to-parameter ratio = 17.3

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



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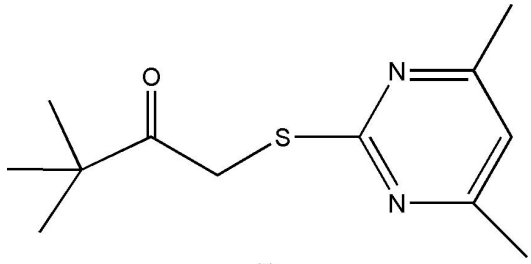
In the title molecule, $C_{12}H_{18}N_2OS$, all bond lengths and angles are normal. The non-H atoms of the 4,6-dimethylpyrimidin-2-ylsulfanyl moiety are coplanar. In the crystal structure, the pyrimidine rings form stacks along the *c* axis with a short interplanar distance of 3.35 Å, indicating the presence of π–π stacking interactions.

## Comment

Pyrimidine compounds are highly efficient in the control of powdery mildew (Wang, 1995; Maurer *et al.*, 1990). As a result of their biological activity, these compounds are under intensive study. In a continuation of our search for new biologically active pyrimidine compounds, the title compound, (I), has been synthesized and its crystal structure is reported.




(I)

In (I) (Fig. 1), the bond lengths and angles in the 4,6-dimethylpyrimidin-2-ylsulfanyl moiety (Table 1) are in good agreement with those found in the literature (Jian *et al.*, 2003). Atoms S1/N1/N2/C1–C6 are essentially coplanar, with a maximum displacement from the mean plane of 0.01 Å for C3. In the crystal structure, the pyrimidine rings form stacks along the *c* axis with a short interplanar distance of 3.35 Å, indicating the presence of π–π stacking interactions; these, along with van der Waals forces, stabilize the crystal packing (Fig. 2).

## Experimental

A mixture of 1-bromo-3,3-dimethylbutan-2-one (1.79 g, 0.01 mol), 4,6-dimethyl-2-mercaptopyrimidine (1.4 g, 0.01 mol) and acetone (50 ml) was stirred for 1 h at room temperature. The solution was then filtered, concentrated and purified by recrystallization to afford the title compound (yield 2.05 g, 86%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethyl acetate at room temperature.

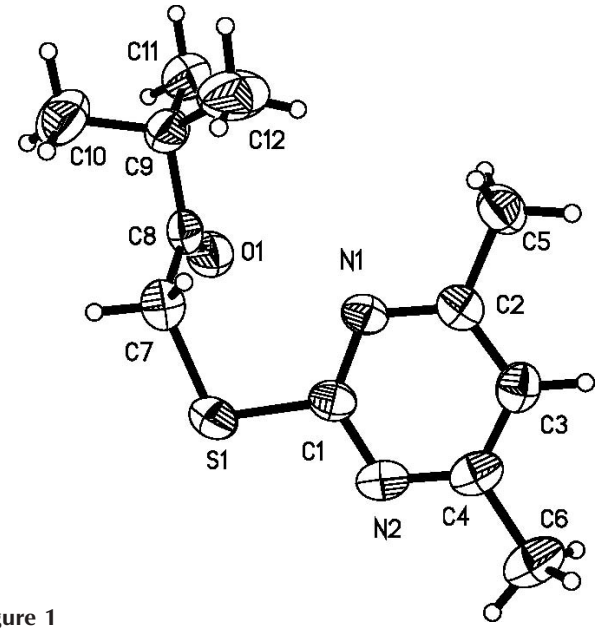



**Figure 1**
View of (I), with 40% probability displacement ellipsoids. Only one component of each of the disordered methyl groups (at atoms C5 and C6) is drawn.

*Crystal data*

| | |
|---|---|
| $C_{12}H_{18}N_2OS$ | $D_x$ = 1.210 Mg m$^{-3}$ |
| $M_r$ = 238.34 | Mo $K\alpha$ radiation |
| Monoclinic, $P2_1/c$ | Cell parameters from 1167 reflections |
| $a$ = 8.8654 (15) Å | $\theta$ = 2.3–19.5° |
| $b$ = 21.938 (4) Å | $\mu$ = 0.23 mm$^{-1}$ |
| $c$ = 6.7526 (12) Å | $T$ = 293 (2) K |
| $\beta$ = 94.967 (2)° | Block, colorless |
| $V$ = 1308.4 (4) Å$^3$ | 0.26 × 0.24 × 0.20 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 2565 independent reflections |
| | 1663 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int}$ = 0.034 |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $\theta_{max}$ = 26.0° |
| | $h = -9 \rightarrow 10$ |
| $T_{min}$ = 0.931, $T_{max}$ = 0.955 | $k = -27 \rightarrow 24$ |
| 7629 measured reflections | $l = -8 \rightarrow 7$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.044 | $w = 1/[\sigma^2(F_o^2) + 0.2819P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.122 | $(\Delta/\sigma)_{max}$ = 0.001 |
| $S$ = 1.03 | $\Delta\rho_{max}$ = 0.20 e Å$^{-3}$ |
| 2565 reflections | $\Delta\rho_{min}$ = −0.30 e Å$^{-3}$ |
| 148 parameters | |

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| S1—C1 | 1.748 (2) | N2—C1 | 1.339 (3) |
| S1—C7 | 1.790 (2) | O1—C8 | 1.203 (3) |
| N1—C1 | 1.329 (2) | C2—C3 | 1.376 (3) |
| N1—C2 | 1.343 (3) | C2—C5 | 1.492 (3) |
| N2—C4 | 1.336 (3) | C3—C4 | 1.375 (3) |
| | | | |
| C1—S1—C7 | 102.33 (11) | C4—N2—C1 | 115.87 (18) |
| C1—N1—C2 | 115.51 (18) | N1—C1—N2 | 127.5 (2) |

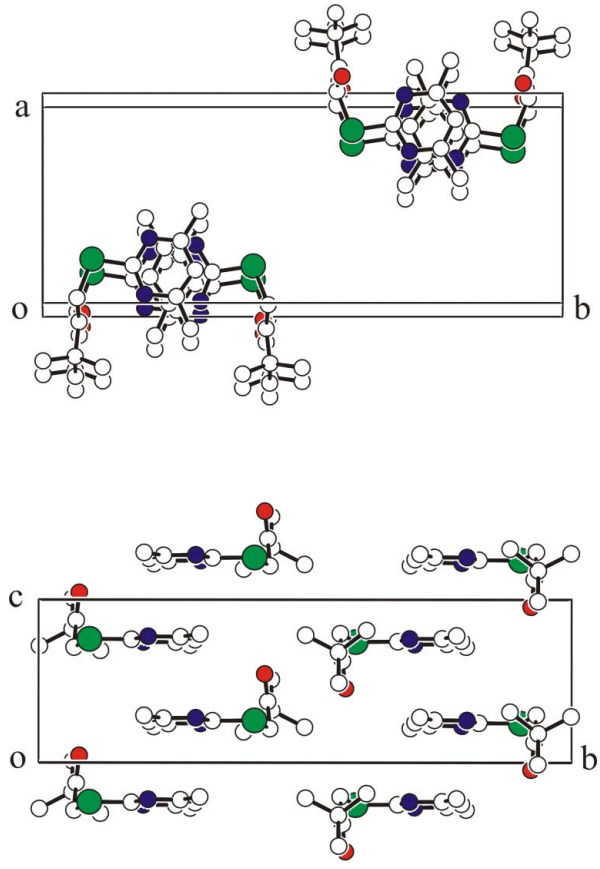



**Figure 2**
The crystal packing of (I), viewed in two orthogonal projections, showing the stacks formed by pyrimidine rings along the *c* axis. H atoms have been omitted for clarity.

All H atoms were placed in calculated positions and included in the final cycles of refinement using a riding model [C—H = 0.93–0.97 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C)]. Two rotationally disordered methyl groups, at atoms C5 and C6, were refined with half site occupancy each.

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) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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