# 2-(4,6-Dimethylpyrimidin-2-ylsulfanyl)-N-(4-methylpyridin-2-yl)acetamide

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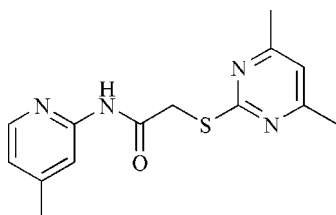
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The non-H atoms of the title molecule, $C_{14}H_{16}N_4OS$, are coplanar, with an r.m.s. deviation of 0.039 Å. The dihedral angle between the two aromatic rings is 2.4 (2)°. An intramolecular C—H···O hydrogen bond is observed. The molecules exist as N—H···N hydrogen-bonded centrosymmetric dimers.

## Related literature

For related literature, see: Koike *et al.* (1999).



## Experimental

### Crystal data

| | |
|---|---|
| $C_{14}H_{16}N_4OS$ | $V$ = 1450.5 (9) Å³ |
| $M_r$ = 288.37 | $Z$ = 4 |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a$ = 5.1924 (19) Å | $\mu$ = 0.22 mm⁻¹ |
| $b$ = 15.423 (5) Å | $T$ = 293 (2) K |
| $c$ = 18.121 (6) Å | 0.40 × 0.24 × 0.20 mm |
| $\beta$ = 91.678 (6)° | |

### Data collection

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 8084 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 1997) | 2970 independent reflections |
| $T_{min}$ = 0.916, $T_{max}$ = 0.957 | 1582 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.060 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.048 | 184 parameters |
| $wR(F^2)$ = 0.144 | H-atom parameters constrained |
| $S$ = 0.98 | $\Delta\rho_{max}$ = 0.27 e Å⁻³ |
| 2970 reflections | $\Delta\rho_{min}$ = −0.23 e Å⁻³ |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3$A$···N4ⁱ | 0.86 | 2.31 | 3.171 (3) | 174 |
| C10—H10···O1 | 0.93 | 2.20 | 2.821 (4) | 123 |

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2528).

## References

Bruker (1997). *SMART* (Version 5.611), *SAINT* (Version 6.0), *SADABS* (Version 2.03) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.

Koike, K., Jia, Z., Nikaido, T., Liu, Y., Zhao, Y. & Guo, D. (1999). *Org. Lett.* **1**, 197–198.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

**supplementary materials**

## 2-(4,6-Dimethylpyrimidin-2-ylsulfanyl)-*N*-(4-methylpyridin-2-yl)acetamide

### D. Liang, L.-X. Gao, Y. Gao, J. Xu and W. Wang

### Comment

Acetamide is an important class of medical intermediate. Many biologically active compounds are prepared by using acetamide (Koike *et al.*, 1999). The title compound was prepared from the reaction of 2-thio-4,6-dimethylpyrimidine with 2-chloro-*N*-(5-methylpyridin-2-yl)acetamide. We report here the crystal structure of the title compound.

The non-hydrogen atoms of the title molecule are coplanar, with an r.m.s. deviation of 0.039 Å. The dihedral angle between the two heterocyclic rings is 2.4 (2)°. The O1—C8—N3 [124.3 (2)°] and N3—C8—C7 [113.9 (2)°] angles deviate significantly from the ideal value of 120°. Due to the *p*-π conjugation bwtween the S atom and the pyrimidine ring, the S1—C1 bond distance [1.756 (3) Å] is slightly shorter than the S1—C7 bond distance [1.794 (3) Å]. An intramolecular C—H···O hydrogen bond is observed. The molecules exist as N—H···O hydrogen-bonded centrosymmetric dimer (Table 1).

### Experimental

The title compound was synthesized by the reaction of 2-thio-4,6-dimethylpyrimidine (2 mmol) with 2-chloro-*N*-(5-methyl-pyridin-2-yl)acetamide (2 mmol) in refluxing ethanol (40 ml). Single crystals suitable for X-ray analysis were grown by slow evaporation of a chloroform-acetone (1:5 *v/v*) solution.

### Refinement

All H atoms were positioned geometrically and refined as riding (N—H = 0.86 Å and C—H = 0.93–0.97 Å). For the CH and CH$_2$ groups, $U_{iso}$(H) values were set equal to 1.2$U_{eq}$(C) and for the methyl groups they were set equal to 1.5$U_{eq}$(C).

### Figures



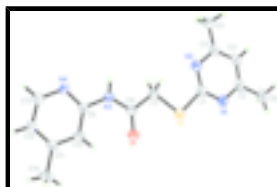Fig. 1. The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

## 2-(4,6-Dimethylpyrimidin-2-ylsulfanyl)-*N*-(4-methylpyridin-2-yl)acetamide

*Crystal data*

| | |
|---|---|
| C$_{14}$H$_{16}$N$_4$OS | $F_{000}$ = 608 |
| $M_r$ = 288.37 | $D_x$ = 1.320 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Melting point: 418 K |

Hall symbol: -P 2ybc

$a = 5.1924$ (19) Å
$b = 15.423$ (5) Å
$c = 18.121$ (6) Å
$\beta = 91.678$ (6)º
$V = 1450.5$ (9) Å$^3$
$Z = 4$

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 1663 reflections
$\theta = 2.6–22.2$º
$\mu = 0.22$ mm$^{-1}$
$T = 293$ (2) K
Plate, colourless
$0.40 \times 0.24 \times 0.20$ mm

*Data collection*

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293(2)$ K

$\varphi$ and $\omega$ scans

Absorption correction: multi-scan (SADABS; Bruker, 1997)

$T_{min} = 0.916$, $T_{max} = 0.957$

8084 measured reflections

2970 independent reflections

1582 reflections with $I > 2\sigma(I)$

$R_{int} = 0.060$

$\theta_{max} = 26.4$º

$\theta_{min} = 1.7$º

$h = -6 \rightarrow 4$

$k = -17 \rightarrow 19$

$l = -22 \rightarrow 22$

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.144$

$S = 0.98$

2970 reflections

184 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0718P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.004$

$\Delta\rho_{max} = 0.27$ e Å$^{-3}$

$\Delta\rho_{min} = -0.23$ e Å$^{-3}$

Extinction correction: none

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit S are based on $F^2$, conventional $R$-factors $R$ are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)*

|      | *x* | *y* | *z* | $U_{iso}*/U_{eq}$ |
|------|-----|-----|-----|-------------------|
| S1   | 0.19772 (16)  | 0.06150 (5)   | 0.30190 (4)   | 0.0565 (3)  |
| O1   | 0.4584 (4)    | 0.17627 (12)  | 0.39721 (11)  | 0.0629 (6)  |
| C8   | 0.5502 (6)    | 0.10500 (16)  | 0.40685 (14)  | 0.0424 (7)  |
| N3   | 0.7497 (4)    | 0.08705 (13)  | 0.45581 (11)  | 0.0437 (6)  |
| H3A  | 0.7929        | 0.0334        | 0.4603        | 0.052*      |
| N1   | −0.0905 (5)   | −0.02849 (15) | 0.21206 (12)  | 0.0526 (6)  |
| N2   | 0.2279 (4)    | −0.11038 (14) | 0.28121 (12)  | 0.0487 (6)  |
| N4   | 1.0824 (5)    | 0.11059 (13)  | 0.54011 (12)  | 0.0471 (6)  |
| C7   | 0.4517 (5)    | 0.02656 (16)  | 0.36422 (15)  | 0.0466 (7)  |
| H7A  | 0.3873        | −0.0166       | 0.3980        | 0.056*      |
| H7B  | 0.5901        | 0.0008        | 0.3369        | 0.056*      |
| C1   | 0.1057 (6)    | −0.03772 (17) | 0.26160 (15)  | 0.0464 (7)  |
| C9   | 0.8914 (5)    | 0.14679 (15)  | 0.49939 (13)  | 0.0390 (7)  |
| C10  | 0.8368 (6)    | 0.23511 (16)  | 0.50028 (15)  | 0.0493 (7)  |
| H10  | 0.7006        | 0.2572        | 0.4716        | 0.059*      |
| C3   | −0.0551 (6)   | −0.18068 (19) | 0.19480 (16)  | 0.0566 (8)  |
| H3   | −0.1119       | −0.2310       | 0.1712        | 0.068*      |
| C12  | 1.1828 (6)    | 0.25295 (18)  | 0.58610 (17)  | 0.0580 (8)  |
| H12  | 1.2871        | 0.2874        | 0.6167        | 0.070*      |
| C4   | 0.1449 (6)    | −0.18362 (18) | 0.24637 (16)  | 0.0502 (7)  |
| C2   | −0.1703 (6)   | −0.1016 (2)   | 0.17864 (15)  | 0.0535 (8)  |
| C5   | 0.2828 (6)    | −0.26511 (18) | 0.26755 (19)  | 0.0677 (9)  |
| H5A  | 0.4476        | −0.2663       | 0.2449        | 0.102*      |
| H5B  | 0.1828        | −0.3142       | 0.2511        | 0.102*      |
| H5C  | 0.3067        | −0.2673       | 0.3202        | 0.102*      |
| C13  | 1.2229 (6)    | 0.16531 (18)  | 0.58239 (17)  | 0.0611 (9)  |
| H13  | 1.3570        | 0.1421        | 0.6112        | 0.073*      |
| C6   | −0.3885 (7)   | −0.0931 (2)   | 0.12243 (18)  | 0.0747 (10) |
| H6A  | −0.5028       | −0.0478       | 0.1372        | 0.112*      |
| H6B  | −0.4812       | −0.1469       | 0.1191        | 0.112*      |
| H6C  | −0.3205       | −0.0792       | 0.0752        | 0.112*      |
| C11  | 0.9856 (6)    | 0.28937 (17)  | 0.54384 (15)  | 0.0507 (8)  |
| C14  | 0.9279 (7)    | 0.38546 (17)  | 0.54669 (19)  | 0.0782 (11) |
| H14A | 0.8268        | 0.3977        | 0.5890        | 0.117*      |
| H14B | 0.8337        | 0.4023        | 0.5026        | 0.117*      |
| H14C | 1.0866        | 0.4173        | 0.5503        | 0.117*      |

*Atomic displacement parameters ($Å^2$)*

|      | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|------|----------|----------|----------|----------|----------|----------|
| S1   | 0.0590 (5)  | 0.0408 (4)  | 0.0681 (5)  | 0.0027 (4)  | −0.0256 (4)  | −0.0038 (4)  |
| O1   | 0.0813 (16) | 0.0368 (11) | 0.0683 (13) | 0.0118 (10) | −0.0348 (12) | −0.0053 (9)  |
| C8   | 0.0517 (18) | 0.0305 (15) | 0.0445 (16) | 0.0044 (13) | −0.0055 (14) | −0.0006 (12) |
| N3   | 0.0501 (15) | 0.0285 (11) | 0.0516 (14) | 0.0060 (10) | −0.0152 (12) | −0.0033 (10) |

| | | | | | |
|---|---|---|---|---|---|
| N1 | 0.0499 (16) | 0.0553 (15) | 0.0518 (15) | −0.0103 (12) | −0.0128 (12) | 0.0042 (12) |
| N2 | 0.0498 (16) | 0.0438 (14) | 0.0521 (14) | −0.0044 (11) | −0.0070 (12) | −0.0049 (11) |
| N4 | 0.0469 (15) | 0.0359 (13) | 0.0574 (14) | 0.0054 (11) | −0.0174 (12) | −0.0049 (11) |
| C7 | 0.0497 (18) | 0.0393 (16) | 0.0502 (17) | 0.0008 (13) | −0.0118 (14) | −0.0047 (13) |
| C1 | 0.0471 (18) | 0.0445 (17) | 0.0476 (17) | −0.0084 (13) | −0.0029 (14) | 0.0002 (13) |
| C9 | 0.0419 (17) | 0.0334 (14) | 0.0414 (15) | 0.0019 (12) | −0.0031 (13) | −0.0014 (12) |
| C10 | 0.0582 (19) | 0.0341 (15) | 0.0546 (18) | 0.0111 (13) | −0.0154 (15) | −0.0024 (13) |
| C3 | 0.060 (2) | 0.0498 (19) | 0.0594 (19) | −0.0169 (16) | −0.0021 (16) | −0.0065 (15) |
| C12 | 0.062 (2) | 0.0379 (17) | 0.072 (2) | −0.0005 (14) | −0.0252 (17) | −0.0088 (14) |
| C4 | 0.0496 (19) | 0.0465 (17) | 0.0544 (18) | −0.0109 (14) | −0.0015 (15) | −0.0074 (14) |
| C2 | 0.0496 (19) | 0.063 (2) | 0.0477 (18) | −0.0202 (16) | −0.0086 (15) | 0.0012 (14) |
| C5 | 0.075 (2) | 0.0444 (18) | 0.083 (2) | −0.0057 (16) | −0.0081 (19) | −0.0105 (16) |
| C13 | 0.057 (2) | 0.0455 (18) | 0.079 (2) | 0.0046 (15) | −0.0272 (17) | −0.0055 (15) |
| C6 | 0.071 (2) | 0.081 (2) | 0.070 (2) | −0.0275 (19) | −0.0276 (19) | 0.0112 (18) |
| C11 | 0.062 (2) | 0.0339 (15) | 0.0554 (18) | 0.0007 (14) | −0.0062 (16) | −0.0046 (13) |
| C14 | 0.104 (3) | 0.0346 (17) | 0.094 (3) | 0.0064 (17) | −0.028 (2) | −0.0098 (16) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—C1 | 1.756 (3) | C3—C2 | 1.386 (4) |
| S1—C7 | 1.794 (3) | C3—H3 | 0.93 |
| O1—C8 | 1.209 (3) | C12—C13 | 1.369 (4) |
| C8—N3 | 1.372 (3) | C12—C11 | 1.380 (4) |
| C8—C7 | 1.516 (3) | C12—H12 | 0.93 |
| N3—C9 | 1.407 (3) | C4—C5 | 1.491 (4) |
| N3—H3A | 0.86 | C2—C6 | 1.507 (4) |
| N1—C2 | 1.340 (3) | C5—H5A | 0.96 |
| N1—C1 | 1.346 (3) | C5—H5B | 0.96 |
| N2—C1 | 1.331 (3) | C5—H5C | 0.96 |
| N2—C4 | 1.358 (3) | C13—H13 | 0.93 |
| N4—C9 | 1.341 (3) | C6—H6A | 0.96 |
| N4—C13 | 1.341 (3) | C6—H6B | 0.96 |
| C7—H7A | 0.97 | C6—H6C | 0.96 |
| C7—H7B | 0.97 | C11—C14 | 1.513 (4) |
| C9—C10 | 1.391 (3) | C14—H14A | 0.96 |
| C10—C11 | 1.373 (4) | C14—H14B | 0.96 |
| C10—H10 | 0.93 | C14—H14C | 0.96 |
| C3—C4 | 1.377 (4) | | |
| C1—S1—C7 | 100.72 (13) | N2—C4—C3 | 120.7 (3) |
| O1—C8—N3 | 124.3 (2) | N2—C4—C5 | 116.0 (3) |
| O1—C8—C7 | 121.8 (3) | C3—C4—C5 | 123.3 (3) |
| N3—C8—C7 | 113.9 (2) | N1—C2—C3 | 121.3 (3) |
| C8—N3—C9 | 127.1 (2) | N1—C2—C6 | 116.6 (3) |
| C8—N3—H3A | 116.5 | C3—C2—C6 | 122.1 (3) |
| C9—N3—H3A | 116.5 | C4—C5—H5A | 109.5 |
| C2—N1—C1 | 115.5 (2) | C4—C5—H5B | 109.5 |
| C1—N2—C4 | 115.7 (2) | H5A—C5—H5B | 109.5 |
| C9—N4—C13 | 115.7 (2) | C4—C5—H5C | 109.5 |
| C8—C7—S1 | 108.17 (18) | H5A—C5—H5C | 109.5 |

| | | | |
|---|---|---|---|
| C8—C7—H7A | 110.1 | H5B—C5—H5C | 109.5 |
| S1—C7—H7A | 110.1 | N4—C13—C12 | 124.6 (3) |
| C8—C7—H7B | 110.1 | N4—C13—H13 | 117.7 |
| S1—C7—H7B | 110.1 | C12—C13—H13 | 117.7 |
| H7A—C7—H7B | 108.4 | C2—C6—H6A | 109.5 |
| N2—C1—N1 | 127.8 (2) | C2—C6—H6B | 109.5 |
| N2—C1—S1 | 120.1 (2) | H6A—C6—H6B | 109.5 |
| N1—C1—S1 | 112.1 (2) | C2—C6—H6C | 109.5 |
| N4—C9—C10 | 123.3 (2) | H6A—C6—H6C | 109.5 |
| N4—C9—N3 | 113.7 (2) | H6B—C6—H6C | 109.5 |
| C10—C9—N3 | 123.0 (2) | C10—C11—C12 | 117.8 (2) |
| C11—C10—C9 | 119.5 (2) | C10—C11—C14 | 120.5 (3) |
| C11—C10—H10 | 120.3 | C12—C11—C14 | 121.6 (3) |
| C9—C10—H10 | 120.3 | C11—C14—H14A | 109.5 |
| C4—C3—C2 | 119.0 (3) | C11—C14—H14B | 109.5 |
| C4—C3—H3 | 120.5 | H14A—C14—H14B | 109.5 |
| C2—C3—H3 | 120.5 | C11—C14—H14C | 109.5 |
| C13—C12—C11 | 119.1 (3) | H14A—C14—H14C | 109.5 |
| C13—C12—H12 | 120.5 | H14B—C14—H14C | 109.5 |
| C11—C12—H12 | 120.5 | | |
| | | | |
| O1—C8—N3—C9 | −4.1 (5) | N3—C9—C10—C11 | −179.4 (2) |
| C7—C8—N3—C9 | 175.6 (2) | C1—N2—C4—C3 | −0.5 (4) |
| O1—C8—C7—S1 | 0.8 (4) | C1—N2—C4—C5 | 179.4 (3) |
| N3—C8—C7—S1 | −178.85 (19) | C2—C3—C4—N2 | 0.2 (4) |
| C1—S1—C7—C8 | −177.95 (19) | C2—C3—C4—C5 | −179.7 (3) |
| C4—N2—C1—N1 | 0.6 (4) | C1—N1—C2—C3 | −0.1 (4) |
| C4—N2—C1—S1 | −179.3 (2) | C1—N1—C2—C6 | −179.5 (3) |
| C2—N1—C1—N2 | −0.2 (4) | C4—C3—C2—N1 | 0.1 (5) |
| C2—N1—C1—S1 | 179.6 (2) | C4—C3—C2—C6 | 179.5 (3) |
| C7—S1—C1—N2 | −1.0 (3) | C9—N4—C13—C12 | 0.1 (4) |
| C7—S1—C1—N1 | 179.1 (2) | C11—C12—C13—N4 | −0.1 (5) |
| C13—N4—C9—C10 | −0.5 (4) | C9—C10—C11—C12 | −0.9 (4) |
| C13—N4—C9—N3 | 179.8 (2) | C9—C10—C11—C14 | −179.1 (3) |
| C8—N3—C9—N4 | −177.6 (2) | C13—C12—C11—C10 | 0.5 (5) |
| C8—N3—C9—C10 | 2.8 (4) | C13—C12—C11—C14 | 178.7 (3) |
| N4—C9—C10—C11 | 0.9 (4) | | |

*Hydrogen-bond geometry (Å, °)*

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| N3—H3A⋯N4[i] | 0.86 | 2.31 | 3.171 (3) | 174 |
| C10—H10⋯O1 | 0.93 | 2.20 | 2.821 (4) | 123 |

Symmetry codes: (i) −$x$+2, −$y$, −$z$+1.

**Fig. 1**