Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Dong Liang, Li-Xing Gao, Yan Gao, Jing Xu and Wei Wang*

School of Chemical Engineering, University of Science and Technology Liaoning, Anshan 114051, People's Republic of China
Correspondence e-mail: tju_chemistry@yahoo.com.cn

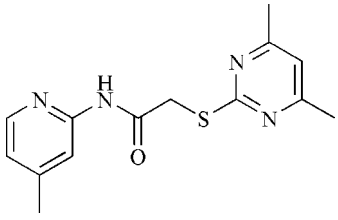
Received 23 November 2007; accepted 28 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.144; data-to-parameter ratio = 16.1.

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

$C_{14}H_{16}N_4OS$
M_r = 288.37
Monoclinic, $P2_1/c$
a = 5.1924 (19) Å
b = 15.423 (5) Å
c = 18.121 (6) Å
β = 91.678 (6)°
V = 1450.5 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 293 (2) K
0.40 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
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

Refinement

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N4^{i}	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.

supporting information

Acta Cryst. (2008). E**64**, o201 [https://doi.org/10.1107/S1600536807064082]

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

Dong Liang, Li-Xing Gao, Yan Gao, Jing Xu and Wei Wang

S1. 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).

S2. Experimental

The title compound was synthesized by the reaction of 2-thio-4,6-dimethylpyrimidine (2 mmol) with 2-chloro-*N*-(5-methylpyridin-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.

S3. 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 1.2U_{eq}(C) and for the methyl groups they were set equal to 1.5U_{eq}(C).

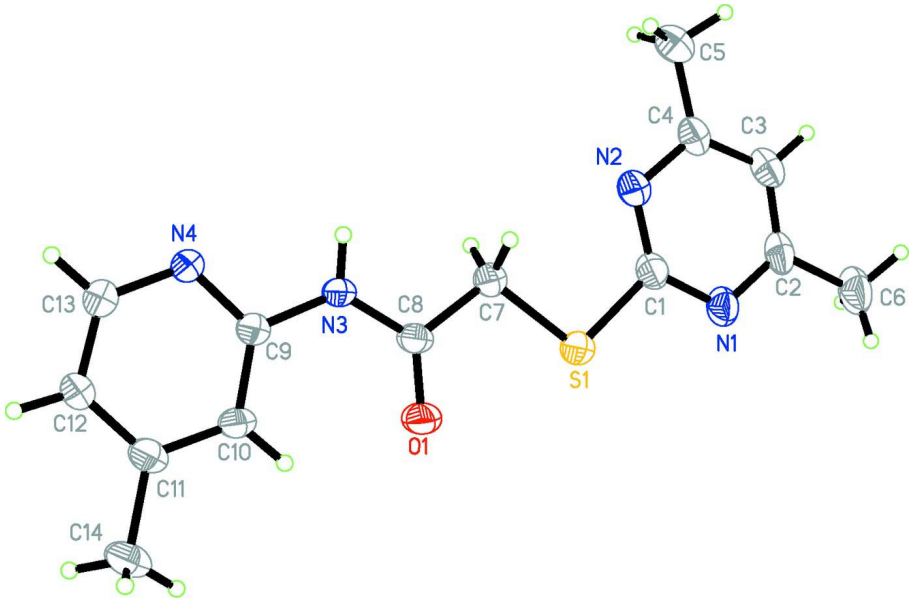


Figure 1

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

$C_{14}H_{16}N_4OS$
$M_r = 288.37$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.1924\ (19)$ Å
$b = 15.423\ (5)$ Å
$c = 18.121\ (6)$ Å
$\beta = 91.678\ (6)°$
$V = 1450.5\ (9)$ Å^3
$Z = 4$

$F(000) = 608$
$D_x = 1.320$ Mg m^{-3}
Melting point: 418 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1663 reflections
$\theta = 2.6–22.2°$
$\mu = 0.22$ mm^{-1}
$T = 293$ K
Plate, colourless
0.40 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω 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 $I > 2\sigma(I)$
$R_{int} = 0.060$
$\theta_{max} = 26.4°$, $\theta_{min} = 1.7°$
$h = -6\rightarrow4$
$k = -17\rightarrow19$
$l = -22\rightarrow22$

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
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0718P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} = 0.004$
H-atom parameters constrained	$\Delta\rho_{max} = 0.27$ e Å^{-3}
	$\Delta\rho_{min} = -0.23$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	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 (Å²)

	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, º)

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, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N4^{i}	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.