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N-(4,6-Dimethylpyrimidin-2-yl)-1,3-benzothiazol-2-amine

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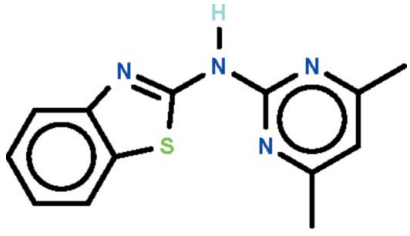
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.126; data-to-parameter ratio = 16.0.

In the title compound, $C_{13}H_{12}N_4S$, an amino N atom is connected to a 1,3-benzothiazole fused-ring system and a dimethyl-substituted pyrimidine ring, these components being aligned [interplanar dihedral angle = 1.9 (1)°]. The secondary amino N atom forms an intermolecular N—H···N hydrogen bond to an N atom of the fused ring of an adjacent molecule, generating a centrosymmetric cyclic hydrogen-bonded dimer [graph set $R_2^2(8)$].

Related literature

For the structure of *N*-(4,6-dimethylpyrimidin-2-yl)-1*H*-benzimidazol-2-amine, see: Mohamed *et al.* (2011). For graph-set analysis, see: Etter *et al.* (1990).



Experimental

Crystal data

$C_{13}H_{12}N_4S$ M_r = 256.34
Monoclinic, $P2_1/n$
a = 6.7608 (2) Å
b = 8.5154 (2) Å
c = 20.6503 (9) Å
β = 97.237 (2)°
V = 1179.39 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 120 K
0.24 × 0.14 × 0.08 mm

Data collection

Bruker–Nonius Roper CCD camera on κ-goniostat diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.940, T_{max} = 0.980
11943 measured reflections
2704 independent reflections
2100 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.126
S = 1.02
2704 reflections
169 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N1^{i}	0.89 (3)	2.27 (3)	3.142 (2)	168 (2)

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2156).

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supporting information

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N-(4,6-Dimethylpyrimidin-2-yl)-1,3-benzothiazol-2-amine

Shaaban K. Mohamed, Peter N. Horton, Mahmoud A. A. El-Remaily, Hussam Abdel-Ghany and Seik Weng Ng

S1. Comment

In an earlier study, we reported the structure of N-(4,6-dimethylpyrimidin-2-yl)-1H-benzimidazol-2-amine (Mohamed et al., 2011). The benzimidazole portion of that molecule was replaced by a benzothiazole unit in the present study, giving the title compound $C_{13}H_{12}N_4S$ (Scheme I). In this molecule, an amino N atom is connected to a benzothiazole fused-ring system and a dimethyl-substituted pyrimidine ring, these being aligned [inter-ring dihedral angle, 1.9 (1)°] (Fig. 1). The amino N atom forms an intermolecular N—H···N hydrogen bond to the N atom of the fused-ring of an adjacent molecule (Table 1) to generate a centrosymmetric cyclic hydrogen-bonded dimer [graph set R</i<>$^2_2$(8) (Etter et al., 1990)].

S2. Experimental

2-(1,3-Benzothiazol-2-yl)guanidine (0.05 mol) was heated in acetylacetone solution (0.10 mol, approx. 10 ml) in the presence of a few drops of acetic acid at 473 K for 1 h. The mixture was cooled and the product was collected and recrystalized from ethanol to give the title compound (m.p. 513 K) in 85% yield.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H, 0.95 to 0.98 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2 to 1.5U_{eq}(C). The amino H-atom was located in a difference Fourier map, and was freely refined. The reflections (-1 2 3) and (0 1 2) were omitted because to bad agreement.

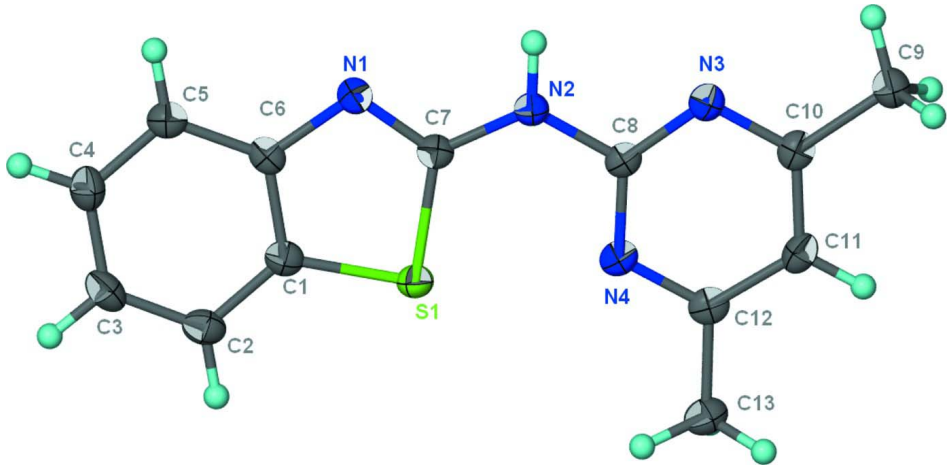

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{13}H_{12}N_4S$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

N-(4,6-Dimethylpyrimidin-2-yl)-1,3-benzothiazol-2-amine

Crystal data

$C_{13}H_{12}N_4S$
$M_r = 256.34$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 6.7608$ (2) Å
$b = 8.5154$ (2) Å
$c = 20.6503$ (9) Å
$\beta = 97.237$ (2)°
$V = 1179.39$ (7) Å^3
$Z = 4$
$F(000) = 536$
$D_x = 1.444$ Mg m^{-3}
Melting point: 513 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2630 reflections
$\theta = 2.9$–$27.5°$
$\mu = 0.26$ mm^{-1}
$T = 120$ K
Block, colorless
0.24 × 0.14 × 0.08 mm

Data collection

Bruker–Nonius Roper CCD camera on κ-goniostat diffractometer
Radiation source: Bruker–Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.940$, $T_{max} = 0.980$
11943 measured reflections
2704 independent reflections
2100 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 27.6°$, $\theta_{min} = 3.1°$
$h = -8 \rightarrow 8$
$k = -11 \rightarrow 10$
$l = -25 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.126$
$S = 1.02$
2704 reflections
169 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 0.7927P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.47670 (7)	0.76071 (6)	0.65817 (3)	0.01754 (17)
N1	0.6118 (2)	0.55355 (17)	0.58054 (8)	0.0158 (4)
N2	0.2981 (2)	0.64918 (19)	0.53944 (9)	0.0170 (4)
H2	0.305 (4)	0.586 (3)	0.5054 (13)	0.034 (7)*
N3	−0.0130 (2)	0.71820 (18)	0.48927 (8)	0.0165 (4)
N4	0.1226 (2)	0.83658 (18)	0.59065 (8)	0.0167 (4)
C1	0.7100 (3)	0.6766 (2)	0.68212 (10)	0.0167 (4)
C2	0.8414 (3)	0.7057 (2)	0.73865 (10)	0.0203 (5)
H2A	0.8097	0.7796	0.7702	0.024*
C3	1.0194 (3)	0.6232 (2)	0.74717 (10)	0.0226 (5)
H3	1.1108	0.6402	0.7854	0.027*

C4	1.0668 (3)	0.5154 (2)	0.70042 (10)	0.0215 (5)
H4	1.1898	0.4602	0.7075	0.026*
C5	0.9374 (3)	0.4875 (2)	0.64396 (10)	0.0184 (4)
H5	0.9708	0.4147	0.6122	0.022*
C6	0.7561 (3)	0.5692 (2)	0.63488 (10)	0.0160 (4)
C7	0.4608 (3)	0.6453 (2)	0.58687 (10)	0.0152 (4)
C8	0.1274 (3)	0.7392 (2)	0.54049 (10)	0.0150 (4)
C9	−0.3381 (3)	0.7869 (2)	0.43244 (11)	0.0201 (4)
H9A	−0.2945	0.7105	0.4017	0.030*
H9B	−0.3627	0.8884	0.4105	0.030*
H9C	−0.4611	0.7497	0.4479	0.030*
C10	−0.1786 (3)	0.8053 (2)	0.48952 (10)	0.0168 (4)
C11	−0.2001 (3)	0.9088 (2)	0.54009 (10)	0.0181 (4)
H11	−0.3180	0.9694	0.5400	0.022*
C12	−0.0455 (3)	0.9217 (2)	0.59088 (10)	0.0168 (4)
C13	−0.0551 (3)	1.0316 (2)	0.64689 (11)	0.0217 (5)
H13A	0.0326	0.9934	0.6851	0.032*
H13B	−0.1924	1.0371	0.6573	0.032*
H13C	−0.0117	1.1364	0.6351	0.032*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0175 (3)	0.0186 (3)	0.0166 (3)	0.00010 (19)	0.0027 (2)	−0.00291 (19)
N1	0.0172 (8)	0.0131 (8)	0.0166 (9)	−0.0006 (6)	0.0008 (7)	0.0007 (6)
N2	0.0170 (9)	0.0173 (8)	0.0163 (9)	0.0018 (7)	0.0008 (7)	−0.0029 (7)
N3	0.0158 (8)	0.0159 (8)	0.0181 (9)	−0.0013 (6)	0.0033 (7)	0.0016 (7)
N4	0.0183 (8)	0.0145 (8)	0.0181 (9)	−0.0003 (6)	0.0051 (7)	0.0009 (7)
C1	0.0189 (10)	0.0165 (9)	0.0153 (10)	−0.0022 (8)	0.0040 (8)	0.0017 (8)
C2	0.0241 (11)	0.0222 (10)	0.0152 (11)	−0.0031 (8)	0.0048 (9)	−0.0002 (8)
C3	0.0240 (11)	0.0272 (11)	0.0153 (11)	−0.0037 (9)	−0.0021 (9)	0.0023 (8)
C4	0.0188 (10)	0.0229 (10)	0.0221 (12)	0.0016 (8)	−0.0002 (9)	0.0044 (9)
C5	0.0212 (10)	0.0164 (9)	0.0180 (11)	−0.0012 (8)	0.0038 (8)	0.0005 (8)
C6	0.0179 (10)	0.0145 (9)	0.0153 (10)	−0.0035 (7)	0.0011 (8)	0.0022 (8)
C7	0.0168 (10)	0.0131 (9)	0.0160 (10)	−0.0025 (7)	0.0027 (8)	−0.0001 (7)
C8	0.0160 (9)	0.0129 (9)	0.0167 (11)	−0.0014 (7)	0.0047 (8)	0.0014 (7)
C9	0.0189 (10)	0.0208 (10)	0.0203 (11)	−0.0001 (8)	0.0013 (9)	0.0012 (8)
C10	0.0175 (9)	0.0133 (9)	0.0201 (11)	−0.0017 (7)	0.0044 (8)	0.0042 (8)
C11	0.0164 (10)	0.0166 (9)	0.0222 (11)	0.0021 (8)	0.0060 (8)	0.0039 (8)
C12	0.0199 (10)	0.0131 (9)	0.0184 (11)	−0.0033 (7)	0.0065 (8)	0.0028 (8)
C13	0.0233 (11)	0.0188 (10)	0.0238 (12)	−0.0001 (8)	0.0068 (9)	−0.0030 (8)

Geometric parameters (Å, º)

S1—C1	1.746 (2)	C3—H3	0.9500
S1—C7	1.762 (2)	C4—C5	1.387 (3)
N1—C7	1.305 (2)	C4—H4	0.9500
N1—C6	1.397 (2)	C5—C6	1.401 (3)

N2—C7	1.378 (2)	C5—H5	0.9500
N2—C8	1.388 (2)	C9—C10	1.502 (3)
N2—H2	0.89 (3)	C9—H9A	0.9800
N3—C8	1.342 (3)	C9—H9B	0.9800
N3—C10	1.343 (2)	C9—H9C	0.9800
N4—C8	1.330 (3)	C10—C11	1.388 (3)
N4—C12	1.349 (3)	C11—C12	1.389 (3)
C1—C6	1.400 (3)	C11—H11	0.9500
C1—C2	1.397 (3)	C12—C13	1.496 (3)
C2—C3	1.385 (3)	C13—H13A	0.9800
C2—H2A	0.9500	C13—H13B	0.9800
C3—C4	1.399 (3)	C13—H13C	0.9800

C1—S1—C7	88.04 (9)	N1—C7—S1	116.81 (14)
C7—N1—C6	109.77 (16)	N2—C7—S1	122.68 (15)
C7—N2—C8	126.35 (18)	N4—C8—N3	127.80 (18)
C7—N2—H2	115.6 (16)	N4—C8—N2	117.28 (17)
C8—N2—H2	118.1 (16)	N3—C8—N2	114.91 (17)
C8—N3—C10	115.50 (17)	C10—C9—H9A	109.5
C8—N4—C12	116.16 (17)	C10—C9—H9B	109.5
C6—C1—C2	121.59 (18)	H9A—C9—H9B	109.5
C6—C1—S1	110.06 (15)	C10—C9—H9C	109.5
C2—C1—S1	128.35 (16)	H9A—C9—H9C	109.5
C3—C2—C1	117.85 (19)	H9B—C9—H9C	109.5
C3—C2—H2A	121.1	N3—C10—C11	121.32 (18)
C1—C2—H2A	121.1	N3—C10—C9	117.08 (18)
C2—C3—C4	121.07 (19)	C11—C10—C9	121.60 (18)
C2—C3—H3	119.5	C10—C11—C12	118.60 (18)
C4—C3—H3	119.5	C10—C11—H11	120.7
C5—C4—C3	121.16 (19)	C12—C11—H11	120.7
C5—C4—H4	119.4	N4—C12—C11	120.60 (18)
C3—C4—H4	119.4	N4—C12—C13	117.25 (18)
C4—C5—C6	118.41 (19)	C11—C12—C13	122.14 (18)
C4—C5—H5	120.8	C12—C13—H13A	109.5
C6—C5—H5	120.8	C12—C13—H13B	109.5
C1—C6—N1	115.32 (17)	H13A—C13—H13B	109.5
C1—C6—C5	119.92 (18)	C12—C13—H13C	109.5
N1—C6—C5	124.76 (18)	H13A—C13—H13C	109.5
N1—C7—N2	120.51 (18)	H13B—C13—H13C	109.5

C7—S1—C1—C6	−0.08 (15)	C8—N2—C7—S1	−0.8 (3)
C7—S1—C1—C2	179.4 (2)	C1—S1—C7—N1	−0.22 (16)
C6—C1—C2—C3	−0.8 (3)	C1—S1—C7—N2	179.59 (17)
S1—C1—C2—C3	179.75 (16)	C12—N4—C8—N3	1.7 (3)
C1—C2—C3—C4	0.6 (3)	C12—N4—C8—N2	−179.41 (16)
C2—C3—C4—C5	0.1 (3)	C10—N3—C8—N4	−0.8 (3)
C3—C4—C5—C6	−0.5 (3)	C10—N3—C8—N2	−179.65 (16)
C2—C1—C6—N1	−179.22 (17)	C7—N2—C8—N4	3.1 (3)

S1—C1—C6—N1	0.3 (2)	C7—N2—C8—N3	−177.90 (17)
C2—C1—C6—C5	0.4 (3)	C8—N3—C10—C11	−0.4 (3)
S1—C1—C6—C5	179.93 (15)	C8—N3—C10—C9	179.09 (17)
C7—N1—C6—C1	−0.5 (2)	N3—C10—C11—C12	0.4 (3)
C7—N1—C6—C5	179.94 (18)	C9—C10—C11—C12	−179.04 (18)
C4—C5—C6—C1	0.3 (3)	C8—N4—C12—C11	−1.6 (3)
C4—C5—C6—N1	179.82 (18)	C8—N4—C12—C13	179.75 (17)
C6—N1—C7—N2	−179.37 (17)	C10—C11—C12—N4	0.6 (3)
C6—N1—C7—S1	0.4 (2)	C10—C11—C12—C13	179.24 (18)
C8—N2—C7—N1	179.05 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N1^{i}	0.89 (3)	2.27 (3)	3.142 (2)	168 (2)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.