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(*E*)-*N*′-[1-(Thiophen-2-yl)ethylidene]-isonicotinohydrazide

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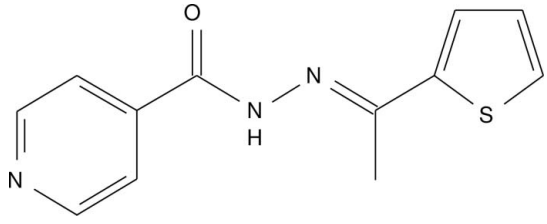
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.104; data-to-parameter ratio = 15.4.

In the title compound, $C_{12}H_{11}N_3OS$, the dihedral angle between the pyridine and thiophene rings is 46.70 (9)° and the C—N—N—C torsion angle is 178.61 (15)°. In the crystal, inversion dimers linked by pairs of N—H···O hydrogen bonds generate $R_2^2(8)$ loops.

Related literature

For a related structure, see: Lu *et al.* (1996). For graph-set nomenclature of hydrogen bonds, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{12}H_{11}N_3OS$
M_r = 245.30
Triclinic, $P\overline{1}$
a = 3.9466 (1) Å
b = 10.5956 (4) Å
c = 14.3647 (6) Å
α = 74.656 (2)°
β = 82.595 (2)°
γ = 79.426 (2)°
V = 567.39 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 293 K
0.30 × 0.28 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.853, T_{max} = 0.935
10651 measured reflections
2456 independent reflections
2162 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.104
S = 1.05
2456 reflections
159 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.89 (1)	2.08 (1)	2.9561 (17)	170 (2)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6959).

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Lu, Z.-L., Duan, C.-Y., Tian, Y.-P., You, X.-Z., Fun, H.-K. & Sivakumar, K. (1996). *Acta Cryst.* C**52**, 1507–1509.
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supporting information

Acta Cryst. (2012). E**68**, o2972 [https://doi.org/10.1107/S1600536812039426]

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S1. Comment

The geometry of C6 atom is distorted trigonal planar geometry as indicated by bond angles O1—C6—N2 = 120.77 (15) Å, (O1—C6—C7) = 119.27 (14) Å, (N2—C6—C7) = 119.96 (13) Å. The bond length of C6 and C7 = 1.496 (2) Å, which is comparable with an equivalent bond length of 1.506 (3) Å for a compound reported earlier (Lu *et al.*, 1996). The crystal structure exhibits intermolecular hydrogen bonds of the type N—H···O with symmetry codes -*x*, 1 - *y*, 2 - *z*.

S2. Experimental

1.37 g (10 mmol) of isoniazide was dissolved by the addition of 15 ml of ethanol in a round bottomed flask. To this 1.1 ml (10 mmol) of 2-Acetyl-thiophene dissolved in 15 ml of ethanol was added. This solution was refluxed for 5 h with stirring and then the solution was concentrated using rotor vaporizer and dried in vacuo and the product obtained was collected. The purity of the compound was confirmed by the TLC. Colourless blocks were recrystallised from methanol solution.

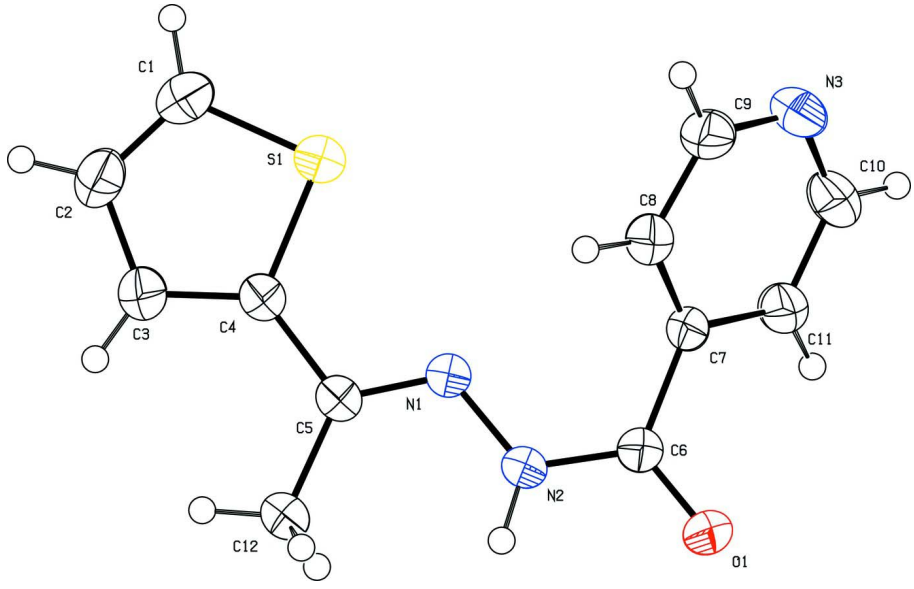

Figure 1

View of the title compound with displacement ellipsoids for non-H atoms drawn at the 50% probability level.

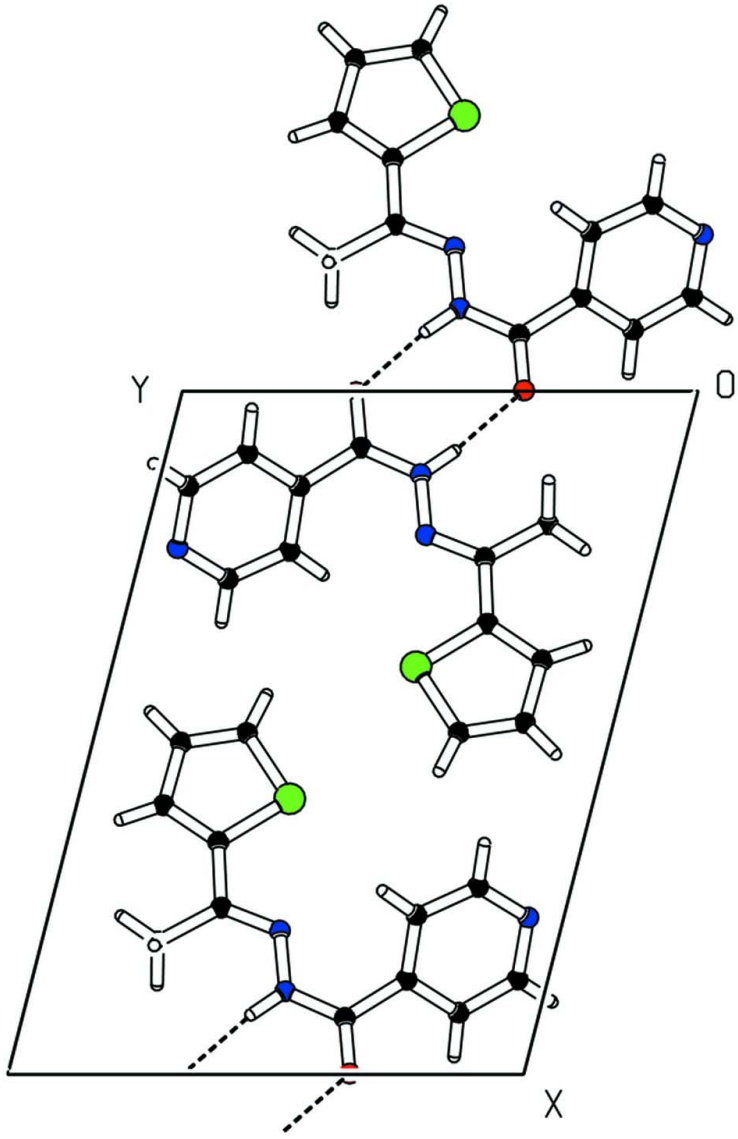

Figure 2

The unit-cell packing diagram.

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$C_{12}H_{11}N_3OS$
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$c = 14.3647\ (6)$ Å
$\alpha = 74.656\ (2)°$
$\beta = 82.595\ (2)°$
$\gamma = 79.426\ (2)°$
$V = 567.39\ (4)$ Å^3
$Z = 2$
$F(000) = 256$
$D_x = 1.436$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5900 reflections
$\theta = 2.2–31.0°$
$\mu = 0.27$ mm^{-1}
$T = 293$ K
Block, colourless
0.30 × 0.28 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.853, T_{max} = 0.935
10651 measured reflections
2456 independent reflections
2162 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 27.0°, θ_{min} = 2.2°
$h = -5 \rightarrow 4$
$k = -13 \rightarrow 13$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.104
S = 1.05
2456 reflections
159 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0524P)^2 + 0.2115P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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}
C1	0.9693 (5)	0.70554 (18)	0.50027 (13)	0.0472 (4)
H1	1.0867	0.6862	0.4441	0.057*
C2	0.8919 (5)	0.82803 (19)	0.51454 (13)	0.0499 (4)
H2	0.9499	0.9031	0.4691	0.060*
C3	0.7129 (5)	0.83102 (17)	0.60598 (12)	0.0446 (4)
H3	0.6397	0.9080	0.6273	0.053*
C4	0.6596 (4)	0.70697 (14)	0.65967 (11)	0.0323 (3)
C5	0.4812 (4)	0.66887 (14)	0.75589 (10)	0.0310 (3)
C6	0.2859 (4)	0.37449 (15)	0.91748 (11)	0.0351 (3)
C7	0.4383 (4)	0.27417 (13)	0.86131 (10)	0.0310 (3)
C8	0.3769 (4)	0.28667 (15)	0.76656 (11)	0.0387 (4)
H8	0.2533	0.3641	0.7313	0.046*
C9	0.5030 (5)	0.18159 (17)	0.72543 (12)	0.0443 (4)
H9	0.4566	0.1904	0.6620	0.053*
C10	0.7437 (5)	0.05892 (16)	0.86100 (14)	0.0483 (4)

H10	0.8728	−0.0189	0.8939	0.058*
C11	0.6241 (4)	0.15680 (15)	0.90973 (12)	0.0400 (4)
H11	0.6679	0.1439	0.9739	0.048*
C12	0.3178 (5)	0.77498 (15)	0.80545 (12)	0.0415 (4)
H12A	0.0709	0.7799	0.8113	0.062*
H12B	0.3787	0.8585	0.7682	0.062*
H12C	0.3985	0.7549	0.8688	0.062*
N1	0.4799 (3)	0.54402 (12)	0.78951 (9)	0.0342 (3)
N2	0.3047 (4)	0.50324 (12)	0.87852 (9)	0.0380 (3)
N3	0.6861 (4)	0.06878 (14)	0.77044 (11)	0.0473 (4)
O1	0.1424 (4)	0.33773 (12)	0.99877 (9)	0.0522 (3)
S1	0.82822 (12)	0.58973 (4)	0.59655 (3)	0.04475 (15)
H2A	0.188 (5)	0.5583 (17)	0.9127 (13)	0.055 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0532 (10)	0.0516 (10)	0.0356 (8)	−0.0122 (8)	0.0064 (7)	−0.0107 (7)
C2	0.0639 (12)	0.0450 (10)	0.0392 (9)	−0.0203 (8)	0.0043 (8)	−0.0038 (7)
C3	0.0596 (11)	0.0350 (8)	0.0399 (9)	−0.0144 (7)	0.0031 (7)	−0.0094 (7)
C4	0.0362 (8)	0.0286 (7)	0.0326 (7)	−0.0052 (6)	−0.0022 (6)	−0.0087 (6)
C5	0.0339 (7)	0.0276 (7)	0.0319 (7)	−0.0042 (5)	−0.0020 (6)	−0.0091 (6)
C6	0.0424 (8)	0.0286 (7)	0.0313 (7)	−0.0031 (6)	0.0050 (6)	−0.0074 (6)
C7	0.0346 (7)	0.0259 (7)	0.0311 (7)	−0.0068 (5)	0.0054 (6)	−0.0071 (5)
C8	0.0479 (9)	0.0322 (8)	0.0343 (8)	−0.0059 (6)	−0.0018 (7)	−0.0064 (6)
C9	0.0576 (10)	0.0439 (9)	0.0358 (8)	−0.0150 (8)	0.0013 (7)	−0.0154 (7)
C10	0.0560 (11)	0.0309 (8)	0.0542 (10)	0.0054 (7)	−0.0039 (8)	−0.0122 (7)
C11	0.0502 (9)	0.0327 (8)	0.0344 (8)	−0.0008 (7)	−0.0036 (7)	−0.0075 (6)
C12	0.0523 (10)	0.0300 (7)	0.0415 (8)	−0.0063 (7)	0.0073 (7)	−0.0132 (6)
N1	0.0429 (7)	0.0275 (6)	0.0304 (6)	−0.0052 (5)	0.0051 (5)	−0.0082 (5)
N2	0.0510 (8)	0.0263 (6)	0.0332 (7)	−0.0032 (5)	0.0099 (6)	−0.0099 (5)
N3	0.0562 (9)	0.0377 (7)	0.0514 (9)	−0.0066 (6)	0.0049 (7)	−0.0217 (6)
O1	0.0758 (9)	0.0345 (6)	0.0369 (6)	−0.0040 (6)	0.0215 (6)	−0.0084 (5)
S1	0.0584 (3)	0.0344 (2)	0.0389 (2)	−0.00466 (18)	0.00777 (18)	−0.01196 (17)

Geometric parameters (Å, º)

C1—C2	1.341 (3)	C7—C11	1.381 (2)
C1—S1	1.6977 (18)	C8—C9	1.380 (2)
C1—H1	0.9300	C8—H8	0.9300
C2—C3	1.414 (2)	C9—N3	1.328 (2)
C2—H2	0.9300	C9—H9	0.9300
C3—C4	1.375 (2)	C10—N3	1.323 (2)
C3—H3	0.9300	C10—C11	1.381 (2)
C4—C5	1.458 (2)	C10—H10	0.9300
C4—S1	1.7162 (15)	C11—H11	0.9300
C5—N1	1.2834 (19)	C12—H12A	0.9600
C5—C12	1.492 (2)	C12—H12B	0.9600

C6—O1	1.2270 (18)	C12—H12C	0.9600
C6—N2	1.3425 (19)	N1—N2	1.3745 (17)
C6—C7	1.4956 (19)	N2—H2A	0.888 (9)
C7—C8	1.381 (2)		

C2—C1—S1	112.29 (14)	C7—C8—H8	120.8
C2—C1—H1	123.9	N3—C9—C8	124.36 (16)
S1—C1—H1	123.9	N3—C9—H9	117.8
C1—C2—C3	112.91 (16)	C8—C9—H9	117.8
C1—C2—H2	123.5	N3—C10—C11	124.17 (16)
C3—C2—H2	123.5	N3—C10—H10	117.9
C4—C3—C2	112.15 (15)	C11—C10—H10	117.9
C4—C3—H3	123.9	C7—C11—C10	118.75 (15)
C2—C3—H3	123.9	C7—C11—H11	120.6
C3—C4—C5	128.92 (14)	C10—C11—H11	120.6
C3—C4—S1	110.69 (12)	C5—C12—H12A	109.5
C5—C4—S1	120.38 (11)	C5—C12—H12B	109.5
N1—C5—C4	115.18 (13)	H12A—C12—H12B	109.5
N1—C5—C12	126.20 (14)	C5—C12—H12C	109.5
C4—C5—C12	118.62 (13)	H12A—C12—H12C	109.5
O1—C6—N2	120.77 (14)	H12B—C12—H12C	109.5
O1—C6—C7	119.27 (13)	C5—N1—N2	117.49 (12)
N2—C6—C7	119.96 (13)	C6—N2—N1	120.90 (12)
C8—C7—C11	117.96 (13)	C6—N2—H2A	115.3 (14)
C8—C7—C6	123.76 (13)	N1—N2—H2A	123.7 (14)
C11—C7—C6	117.98 (13)	C10—N3—C9	116.26 (14)
C9—C8—C7	118.49 (15)	C1—S1—C4	91.96 (8)
C9—C8—H8	120.8		

S1—C1—C2—C3	0.1 (2)	C7—C8—C9—N3	−1.2 (3)
C1—C2—C3—C4	0.2 (3)	C8—C7—C11—C10	1.0 (2)
C2—C3—C4—C5	−178.72 (16)	C6—C7—C11—C10	175.01 (15)
C2—C3—C4—S1	−0.3 (2)	N3—C10—C11—C7	−1.4 (3)
C3—C4—C5—N1	−178.08 (16)	C4—C5—N1—N2	−177.77 (13)
S1—C4—C5—N1	3.7 (2)	C12—C5—N1—N2	1.8 (2)
C3—C4—C5—C12	2.3 (3)	O1—C6—N2—N1	176.75 (16)
S1—C4—C5—C12	−175.92 (12)	C7—C6—N2—N1	−3.7 (2)
O1—C6—C7—C8	130.37 (18)	C5—N1—N2—C6	178.61 (15)
N2—C6—C7—C8	−49.1 (2)	C11—C10—N3—C9	0.5 (3)
O1—C6—C7—C11	−43.3 (2)	C8—C9—N3—C10	0.8 (3)
N2—C6—C7—C11	137.23 (16)	C2—C1—S1—C4	−0.23 (16)
C11—C7—C8—C9	0.2 (2)	C3—C4—S1—C1	0.32 (14)
C6—C7—C8—C9	−173.46 (15)	C5—C4—S1—C1	178.87 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N2—H2*A*···O1^{i}	0.89 (1)	2.08 (1)	2.9561 (17)	170 (2)

Symmetry code: (i) −*x*, −*y*+1, −*z*+2.