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Cinnamoylthiourea

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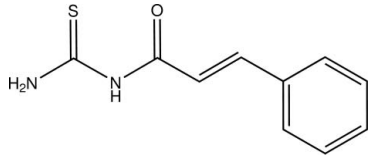
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; R factor = 0.065; wR factor = 0.156; data-to-parameter ratio = 20.1.

In the title compound [systematic name: 1-(3-phenylprop-2-enoyl)thiourea], $C_{10}H_{10}N_2OS$, the acetylthiourea fragment and the phenyl ring adopt an *E* configuration. The roughly planar but-2-enoylthiourea fragment [maximum deviation = 0.053 (3) Å] forms a dihedral of 10.54 (11)° with the phenyl ring. An intramolecular N—H···O hydrogen bond generates an *S*(6) ring. In the crystal, molecules are linked into sheets parallel to (100) by N—H···S hydrogen bonds.

Related literature

For the preparation, see: Hassan *et al.* (2010*a*). For related structures, see: Hung *et al.* (2010); Hassan *et al.* (2008*a*,*b*,*c*, 2009, 2010*a*,*b*); Yamin & Hassan (2004). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{10}H_{10}N_2OS$
M_r = 206.26
Monoclinic, $P2_1/c$
a = 14.3313 (18) Å
b = 4.9801 (6) Å
c = 15.4199 (19) Å
β = 111.612 (3)°
V = 1023.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 273 K
0.34 × 0.12 × 0.09 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.960, T_{max} = 0.975
7192 measured reflections
2551 independent reflections
1688 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.156
S = 1.08
2551 reflections
127 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 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	0.89	1.95	2.649 (3)	134
N1—H1A···S1^{i}	0.85	2.79	3.602 (2)	159
N2—H2B···S1^{ii}	0.88	2.54	3.409 (2)	169

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, -y, -z+1$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5180).

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supporting information

Acta Cryst. (2010). E**66**, o2796 [https://doi.org/10.1107/S1600536810040018]

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S1. Comment

The title compound, (I), is an amide thiourea derivative of cinnamoyl analogous to our previously reported molecules, methyl-2-(3-cinnamoylthioureido)acetate (Hassan *et al.*, 2010*a*) (II), propyl-2-(3-benzoylthioureido)acetate (Hassan *et al.*, 2008*b*) (III), butyl-2-(3-benzoylthioureido)acetate (Hassan *et al.*, 2008*c*) (IV), methyl-2-(3-benzoylthioureido)acetate (Hassan *et al.*, 2009) (V) and ethyl-2-(3-cinnamoylthioureido)acetate (Hassan *et al.*, 2010*b*) (VI). As in most of carbonyl-thiourea derivatives of the type R^1C(O)NHC(S)NHR^2, the molecule maintains the *E*—*Z* configuration with respect to the positions of the cinnamoyl moiety and the hydrogen atom of the terminal amide group, respectively, relative to the S atom across the C10—N2 bond (Fig 1). The bond lengths (Allen *et al.*, 1987) and angles in the molecule are in normal ranges and comparable to those observed in (II), (III), (IV), (V) and (VI). However, the C═S bond length [1.679 (2) Å] is slightly longer than that observed in (II) [1.666 (3) Å]. The S1/O1/N1/N2/C6/C7/C8/C9/C10 fragment is essentially planar with a maximum deviation of 0.053 (3) Å, for atom C8. The C1–C6 phenyl ring is inclined to the above plane with a dihedral angle of 10.54 (11)°, which is smaller than that found in (II) [11.17 (14)°]. There is one intramolecular hydrogen bond, N2—H2A···O1 (Table 1), which resulted in the formation of pseudo-six-membered ring (N2/H2A/O1/C9/N1/C10) (Fig 1). The molecular packing is stablized by two intermolecular hydrogen bonds viz. N1—H1A···S1 and N1—H1A···S1 (Table 1) which form a two-dimensional network parallel to (100) [Fig. 2].

S2. Experimental

The title compound was obtained from a reaction sheme similar to the cinnamoylthiourea ester synthesis starting from 2-(3-cinnamoylthioureido) acetic acid with alcohol in the presence of $LaCl_3$ reported earlier (Hassan *et al.*, 2010*a*). Colourless single crystals, suitable for X-ray analysis, were obtained by slow evaporation of a CH_2Cl_2 solution at room temperature (yield 77%).

S3. Refinement

H atoms of C atoms were positioned geometrically [C–H = 0.93 Å] and allowed to ride on their parent atoms, with U_{iso} = 1.2U_{eq}(C). The H atoms of N atoms were located in difference fouriuor maps and allowed to ride on their parent atoms, with N–H = 0.87 (1) Å and U_{iso} = 1.2U_{eq}(N).

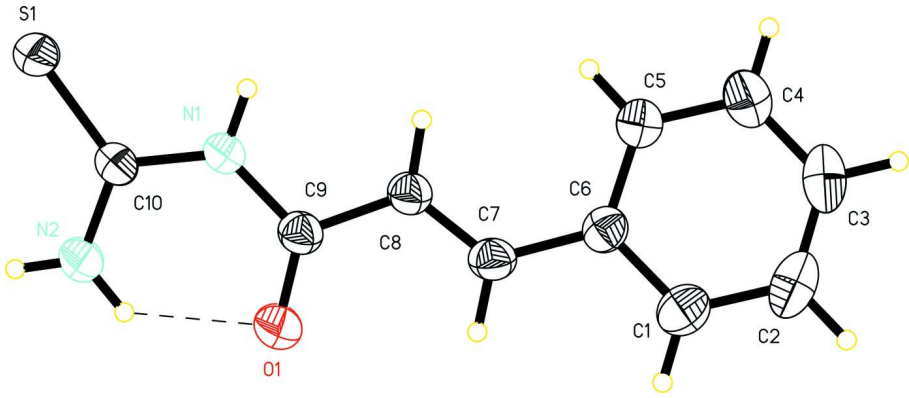

Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

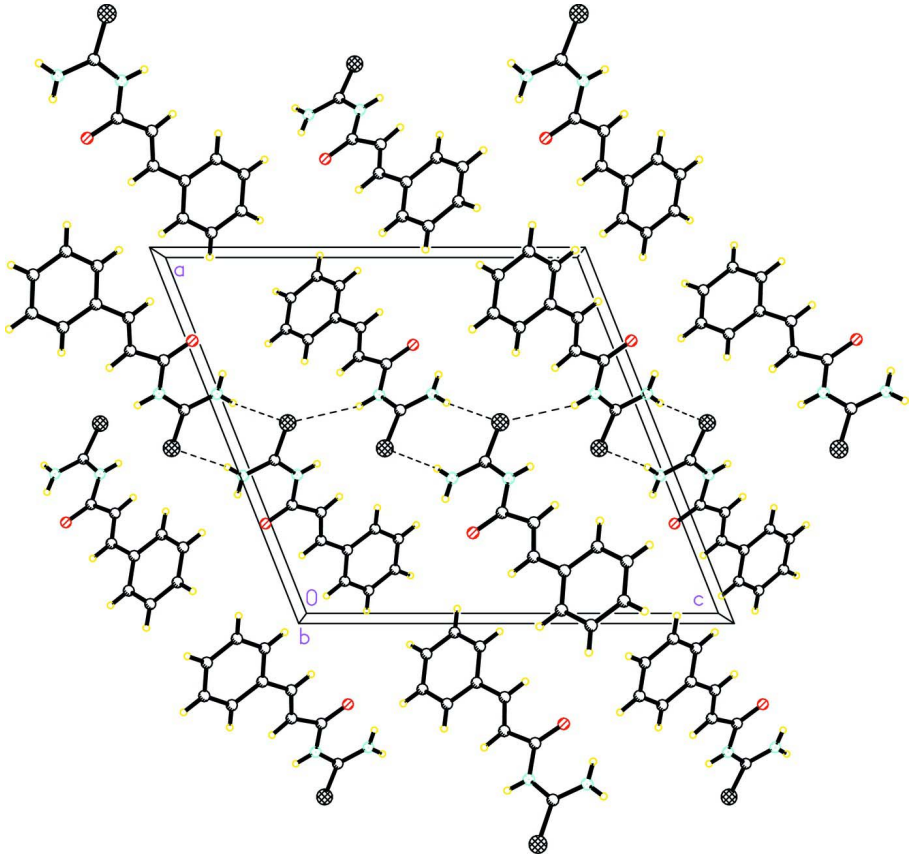

Figure 2

Part of the crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

1-(3-phenylprop-2-enoyl)thiourea

Crystal data

$C_{10}H_{10}N_2OS$
$M_r = 206.26$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

$a = 14.3313\ (18)$ Å
$b = 4.9801\ (6)$ Å
$c = 15.4199\ (19)$ Å
$\beta = 111.612\ (3)°$

V = 1023.2 (2) Å^3
Z = 4
F(000) = 432
D_x = 1.339 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1059 reflections
θ = 1.5–28.3°
μ = 0.28 mm^{-1}
T = 273 K
Plate, colourless
0.34 × 0.12 × 0.09 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.960, T_{max} = 0.975
7192 measured reflections
2551 independent reflections
1688 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 28.3°, θ_{min} = 1.5°
h = −18→19
k = −6→6
l = −20→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.156
S = 1.08
2551 reflections
127 parameters
3 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0703P)^2 + 0.1088P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.40 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	−0.03467 (5)	0.16643 (15)	0.35571 (4)	0.0559 (3)
O1	0.24962 (15)	0.6309 (4)	0.51663 (12)	0.0647 (6)
N1	0.11111 (14)	0.5226 (4)	0.38961 (13)	0.0428 (5)
H1A	0.0790	0.5740	0.3339	0.051*
N2	0.11216 (16)	0.2739 (5)	0.51525 (14)	0.0551 (6)
H2A	0.1680	0.3641	0.5479	0.066*
H2B	0.0850	0.1571	0.5415	0.066*
C1	0.2743 (2)	1.2916 (6)	0.26352 (19)	0.0553 (7)
H1B	0.2112	1.2149	0.2350	0.066*
C2	0.3067 (2)	1.4824 (6)	0.2166 (2)	0.0674 (8)
H2C	0.2655	1.5331	0.1567	0.081*

C3	0.3993 (2)	1.5982 (6)	0.2575 (2)	0.0676 (8)
H3A	0.4206	1.7273	0.2253	0.081*
C4	0.4604 (2)	1.5251 (6)	0.3454 (2)	0.0669 (8)
H4A	0.5232	1.6043	0.3731	0.080*
C5	0.42846 (19)	1.3317 (6)	0.3932 (2)	0.0551 (7)
H5A	0.4704	1.2819	0.4530	0.066*
C6	0.33484 (18)	1.2118 (5)	0.35306 (17)	0.0431 (6)
C7	0.30347 (18)	1.0120 (5)	0.40557 (17)	0.0456 (6)
H7A	0.3462	0.9838	0.4670	0.055*
C8	0.22069 (18)	0.8664 (5)	0.37521 (16)	0.0434 (6)
H8A	0.1758	0.8900	0.3143	0.052*
C9	0.19735 (18)	0.6684 (5)	0.43484 (16)	0.0433 (6)
C10	0.06860 (17)	0.3267 (5)	0.42595 (15)	0.0395 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0556 (4)	0.0654 (5)	0.0402 (4)	−0.0166 (3)	0.0101 (3)	0.0071 (3)
O1	0.0744 (13)	0.0688 (13)	0.0390 (10)	−0.0198 (10)	0.0072 (9)	0.0076 (9)
N1	0.0475 (11)	0.0421 (11)	0.0342 (10)	−0.0031 (9)	0.0097 (9)	0.0060 (9)
N2	0.0651 (14)	0.0608 (15)	0.0354 (11)	−0.0148 (11)	0.0139 (10)	0.0072 (10)
C1	0.0558 (15)	0.0559 (17)	0.0509 (15)	−0.0097 (13)	0.0160 (13)	0.0026 (13)
C2	0.077 (2)	0.065 (2)	0.0623 (18)	−0.0090 (17)	0.0280 (16)	0.0113 (16)
C3	0.081 (2)	0.0569 (18)	0.083 (2)	−0.0114 (16)	0.0516 (19)	0.0027 (17)
C4	0.0598 (17)	0.0601 (19)	0.092 (2)	−0.0174 (15)	0.0407 (18)	−0.0169 (18)
C5	0.0523 (15)	0.0526 (16)	0.0576 (17)	−0.0040 (13)	0.0170 (13)	−0.0088 (14)
C6	0.0444 (12)	0.0373 (13)	0.0470 (14)	−0.0009 (10)	0.0162 (11)	−0.0036 (11)
C7	0.0488 (14)	0.0427 (14)	0.0392 (12)	−0.0002 (11)	0.0090 (11)	−0.0021 (11)
C8	0.0490 (13)	0.0410 (14)	0.0368 (12)	−0.0022 (11)	0.0117 (10)	−0.0003 (11)
C9	0.0504 (13)	0.0408 (14)	0.0369 (13)	−0.0005 (11)	0.0140 (11)	−0.0009 (11)
C10	0.0455 (12)	0.0383 (12)	0.0360 (12)	0.0041 (11)	0.0162 (10)	0.0034 (10)

Geometric parameters (Å, º)

S1—C10	1.679 (2)	C2—H2C	0.93
O1—C9	1.221 (3)	C3—C4	1.365 (4)
N1—C10	1.374 (3)	C3—H3A	0.93
N1—C9	1.381 (3)	C4—C5	1.389 (4)
N1—H1A	0.85	C4—H4A	0.93
N2—C10	1.312 (3)	C5—C6	1.389 (3)
N2—H2A	0.89	C5—H5A	0.93
N2—H2B	0.88	C6—C7	1.455 (3)
C1—C2	1.374 (4)	C7—C8	1.320 (3)
C1—C6	1.391 (3)	C7—H7A	0.93
C1—H1B	0.93	C8—C9	1.468 (3)
C2—C3	1.369 (4)	C8—H8A	0.93
C10—N1—C9	128.04 (19)	C6—C5—C4	121.0 (3)

C10—N1—H1A	118.0	C6—C5—H5A	119.5
C9—N1—H1A	113.7	C4—C5—H5A	119.5
C10—N2—H2A	118.2	C5—C6—C1	117.8 (2)
C10—N2—H2B	119.8	C5—C6—C7	119.5 (2)
H2A—N2—H2B	122.0	C1—C6—C7	122.7 (2)
C2—C1—C6	120.8 (3)	C8—C7—C6	126.9 (2)
C2—C1—H1B	119.6	C8—C7—H7A	116.6
C6—C1—H1B	119.6	C6—C7—H7A	116.6
C3—C2—C1	120.4 (3)	C7—C8—C9	121.9 (2)
C3—C2—H2C	119.8	C7—C8—H8A	119.0
C1—C2—H2C	119.8	C9—C8—H8A	119.0
C4—C3—C2	120.3 (3)	O1—C9—N1	122.4 (2)
C4—C3—H3A	119.9	O1—C9—C8	123.7 (2)
C2—C3—H3A	119.9	N1—C9—C8	113.9 (2)
C3—C4—C5	119.7 (3)	N2—C10—N1	117.3 (2)
C3—C4—H4A	120.1	N2—C10—S1	123.18 (19)
C5—C4—H4A	120.1	N1—C10—S1	119.49 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1	0.89	1.95	2.649 (3)	134
N1—H1*A*···S1^{i}	0.85	2.79	3.602 (2)	159
N2—H2*B*···S1^{ii}	0.88	2.54	3.409 (2)	169

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+1/2; (ii) −*x*, −*y*, −*z*+1.