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Key indicators

Single-crystal X-ray study
 $T = 273\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.045
 wR factor = 0.123
Data-to-parameter ratio = 18.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

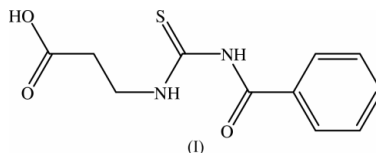
3-(3-Benzoylthioureido)propionic acid

The molecular structure of the title compound, $\text{C}_{11}\text{H}_{12}\text{N}_2\text{O}_3\text{S}$, adopts a *cis-trans* configuration with respect to the position of the benzoyl and propionic acid groups relative to the S atom across the thiourea C—N bonds, respectively. In the crystal structure, the molecules are linked by weak N—H···S, N—H···O and O—H···O interactions to form a two-dimensional network perpendicular to the *a* axis.

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Comment

The molecular dimensions of the title compound, (I), are in agreement with other benzoylthiourea derivatives, PhCONHCSNHR , where $R = \text{Ph}$ (Yamin & Yusof, 2003*a*), $R = p$ -bromophenyl (Yamin & Yusof, 2003*b*) and $R = 3,4$ -dimethylphenyl (Shanmuga Sundara Raj *et al.*, 1999). The title compound adopts a *cis-trans* configuration with respect to the position of the propionic acid and benzoyl groups relative to the S atom across the C8—N2 and C8—N1 bonds, respectively.



The central carbonyl-thiourea moiety (S1/C8/N1/N2/C7), phenyl (C1—C6) and propionic acid [maximum deviation at C9 of -0.130 (2) \AA] fragments are planar. The central thiourea moiety makes angles with the phenyl and propionic acid fragments of 52.74 (9) and 75.14 (11) $^\circ$, respectively. The phenyl ring is inclined to the propionic acid fragment by 22.46 (13) $^\circ$. There is one intramolecular hydrogen bond, N2—H2A···O1 (Table 2) and, as a result, a pseudo-six-membered ring (N2—C8—N1—C7—O1—H2A) is formed. In the crystal structure, the molecules are linked by intermolecular contacts, N2—H2A···O1ⁱ, N1—H1A···S1ⁱⁱ and O3—H3···O2ⁱⁱⁱ (see Table 2 for symmetry codes) to form a two-dimensional network perpendicular to the *a* axis (Fig. 2).

Experimental

A solution of 3-aminopropionic acid (2.22 g, 0.025 mol) in acetone (50 ml) was added dropwise to 50 ml of an acetone solution containing an equimolar amount of benzoyl isothiocyanate in a two-necked round-bottomed flask. The solution was refluxed for about 2 h and then cooled in ice. The white precipitate was filtered off and washed with ethanol–distilled water, then dried in a vacuum (yield 85%). Recrystallization from ethanol yielded single crystals suitable for X-ray analysis.

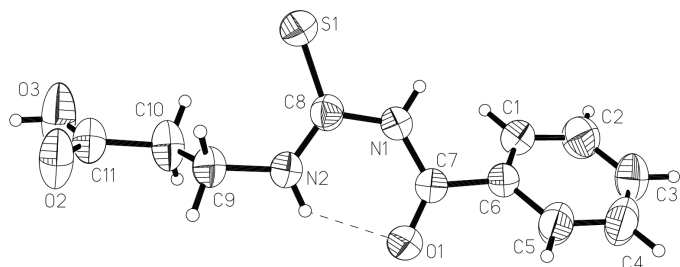


Figure 1
The molecular structure of the title compound, (I), with displacement ellipsoids drawn at the 50% probability level.

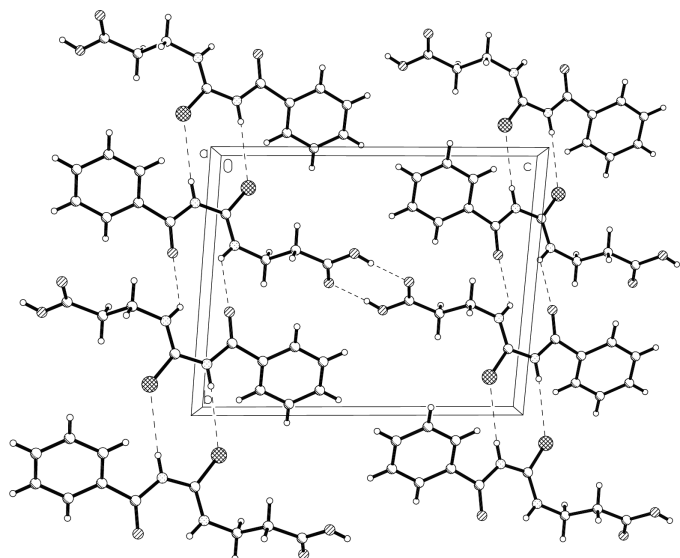


Figure 2
Packing diagram of compound (I), viewed down the *b* axis. The dashed lines denote N—H...S, N—H...O and O—H...O hydrogen bonds.

Crystal data

$C_{11}H_{12}N_2O_3S$
 $M_r = 252.29$
Triclinic, $P\bar{1}$
 $a = 4.5868$ (9) Å
 $b = 10.582$ (2) Å
 $c = 13.080$ (3) Å
 $\alpha = 94.685$ (3)°
 $\beta = 91.341$ (3)°
 $\gamma = 96.759$ (3)°
 $V = 628.0$ (2) Å³

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.866$, $T_{\max} = 0.955$
7220 measured reflections

$Z = 2$
 $D_x = 1.334$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 2840 reflections
 $\theta = 1.6$ – 27.5°
 $\mu = 0.26$ mm⁻¹
 $T = 273$ (2) K
Slab, colourless
 $0.58 \times 0.46 \times 0.18$ mm

2818 independent reflections
2363 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.017$
 $\theta_{\text{max}} = 27.5^\circ$
 $h = -5 \rightarrow 5$
 $k = -13 \rightarrow 13$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.123$
 $S = 1.03$
2818 reflections
155 parameters
H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2 + 0.1496P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.27$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

S1—C8	1.6728 (17)	O3—C11	1.296 (2)
O1—C7	1.222 (2)	N2—C8	1.317 (2)
O2—C11	1.199 (2)	N2—C9	1.454 (2)
C7—N1—C8	127.95 (14)	N2—C8—S1	123.77 (13)
C8—N2—C9	123.27 (15)	N1—C8—S1	118.97 (12)
N2—C8—N1	117.26 (14)		

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H2A...O1	0.86	1.99	2.656 (2)	133
N2—H2A...O1 ⁱ	0.86	2.40	3.047 (2)	132
N1—H1A...S1 ⁱⁱ	0.86	2.69	3.5466 (16)	175
O3—H3...O2 ⁱⁱⁱ	0.82	1.83	2.649 (2)	176

Symmetry codes: (i) $2 - x, 1 - y, -z$; (ii) $1 - x, -y, -z$; (iii) $1 - x, 1 - y, 1 - z$.

After their location in a difference Fourier map, all H atoms were placed geometrically and allowed to ride on their parent C or N atoms with C—H = 0.93–0.97 Å and N—H = 0.86 Å.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 1990).

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