

Nurziana Ngah,* Mohammad B.
Kassim and Bohari M. YaminSchool of Chemical Sciences and Food
Technology, Universiti Kebangsaan Malaysia,
43600 Bangi, Selangor, MalaysiaCorrespondence e-mail:
nurziana_ngah@yahoo.com

Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.037
 wR factor = 0.104
Data-to-parameter ratio = 13.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

2-(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 positions of the propionic acid and benzoyl groups relative to the S atom across the thiourea C—N bonds. In the crystal structure, molecules are linked by $\text{O}-\text{H}\cdots\text{S}$ and $\text{C}-\text{H}\cdots\text{O}$ interactions, forming a one-dimensional chain parallel to the *b* axis.

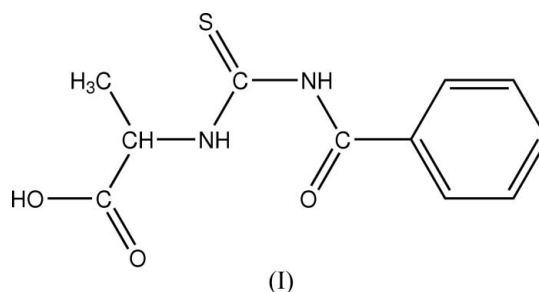
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Comment

The title compound, (I), is isomorphous with 3-(3-benzoylthioureido)propionic acid (Yusof & Yamin, 2003); they differ in that the 3-benzoylthioureido group is attached to the β -alanine group in the latter compound. The molecular structure adopts a *cis-trans* configuration with respect to the positions of the propionic acid and benzoyl groups relative to the S atom across the C8—N2 and C8—N1 bonds, respectively.



The bond lengths and angles (Table 1) are in normal ranges (Allen *et al.*, 1987) and comparable with those in the β -alanine derivative. The central carbonylthiourea group (S1/C8/N1/N2/C7), and the phenyl (C1—C6) and ethanoic acid fragments are planar, with a maximum deviation of 0.037 (2) \AA for atom C7. The central carbonylthiourea group makes dihedral angles

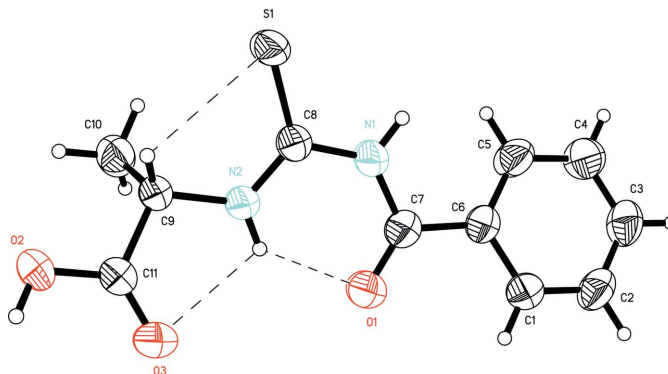


Figure 1

The molecular structure of the title compound, (I), with displacement ellipsoids drawn at the 50% probability level. Dashed lines indicate hydrogen bonds.

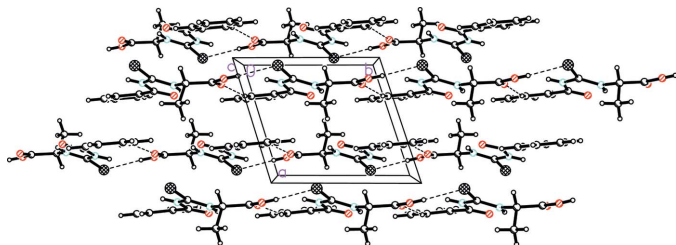


Figure 2
Packing diagram of compound (I), viewed down the *c* axis. The dashed lines denote O—H...S and C—H...O hydrogen bonds.

with the phenyl and ethanoic acid fragments of 27.52 (9) and 24.20 (12)°, respectively. The phenyl ring is inclined to the ethanoic acid fragment by 4.19 (4)°.

There are three intramolecular hydrogen bonds C9—H9...S1, N2—H2A...O1 and N2—H2A...O3 (Table 2) and, as a result, two pseudo-five-membered rings (C9—H9—S1—C8—N2), (N2—H2A—O3—C11—C9) and a pseudo-six-membered ring (N2—H2A—O1—C7—N1—C8) are formed (Fig. 1). In the crystal structure, the molecules are linked by intermolecular contacts, O2—H2...S1ⁱ and C5—H5...O3ⁱⁱ (see Table 2 for symmetry codes), forming a one-dimensional chain parallel to the *b* axis (Fig. 2).

Experimental

A solution of 2-aminopropionic acid (4.45 g, 0.05 mol) in acetone (20 ml) was added dropwise to an acetone solution (20 ml) containing an equimolar amount of benzoyl isothiocyanate in a two-necked round-bottomed flask. The solution was refluxed for about 5 h and then filtered into a beaker containing ice. The yellow precipitate was washed with cold acetone—distilled water, before being dried and kept in a desiccator (yield 10.72 g, 85%, m.p. 430–431 K). Recrystallization from acetonitrile yielded single crystals suitable for X-ray analysis.

Crystal data

C ₁₁ H ₁₂ N ₂ O ₃ S	<i>Z</i> = 2
<i>M_r</i> = 252.29	<i>D_x</i> = 1.419 Mg m ⁻³
Triclinic, <i>P</i> $\bar{1}$	Mo <i>K</i> α radiation
<i>a</i> = 7.3570 (18) Å	Cell parameters from 835 reflections
<i>b</i> = 8.083 (2) Å	<i>θ</i> = 1.9–25.0°
<i>c</i> = 10.706 (3) Å	<i>μ</i> = 0.27 mm ⁻¹
<i>α</i> = 87.395 (4)°	<i>T</i> = 298 (2) K
<i>β</i> = 77.128 (4)°	Block, yellow
<i>γ</i> = 72.065 (5)°	0.49 × 0.33 × 0.31 mm
<i>V</i> = 590.3 (3) Å ³	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2076 independent reflections
<i>ω</i> scans	1858 reflections with <i>I</i> > 2σ(<i>I</i>)
Absorption correction: multi-scan (SADABS; Bruker, 2000)	<i>R_{int}</i> = 0.020
<i>T_{min}</i> = 0.878, <i>T_{max}</i> = 0.920	<i>θ_{max}</i> = 25.0°
5591 measured reflections	<i>h</i> = -8 → 8
	<i>k</i> = -9 → 9
	<i>l</i> = -12 → 12

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.037
wR (*F*²) = 0.104
S = 1.11
 2076 reflections
 156 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.2021P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.21 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.18 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

S1—C8	1.6778 (19)	N1—C8	1.385 (2)
O1—C7	1.212 (2)	N1—C7	1.385 (2)
O2—C11	1.321 (2)	N2—C8	1.315 (2)
O3—C11	1.195 (2)	N2—C9	1.454 (2)
C8—N1—C7	128.30 (16)	N2—C8—S1	123.69 (14)
C8—N2—C9	122.46 (15)	N1—C8—S1	118.56 (14)
N2—C8—N1	117.74 (16)		

Table 2

Hydrogen-bond 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>
C9—H9...S1	0.98	2.67	3.033 (2)	102
N2—H2A...O1	0.86	2.01	2.669 (2)	133
N2—H2A...O3	0.86	2.39	2.698 (2)	102
O2—H2...S1 ⁱ	0.82	2.32	3.1190 (16)	166
C5—H5...O3 ⁱⁱ	0.93	2.30	3.180 (3)	158

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

H atoms were positioned geometrically [O—H = 0.82, N—H = 0.86 and C—H = 0.93 or 0.96 Å (methyl)] and constrained to ride on their parent atoms, with *U*_{iso}(H) = 1.2 (1.5 methyl and hydroxyl) *U*_{eq}(C/N/O).

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); 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, 2003).

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