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# *N*,*N*′-Bis(2-phenylethyl)thiourea

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**Key indicators**

Single-crystal X-ray study
*T* = 173 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.042
*wR* factor = 0.100
Data-to-parameter ratio = 19.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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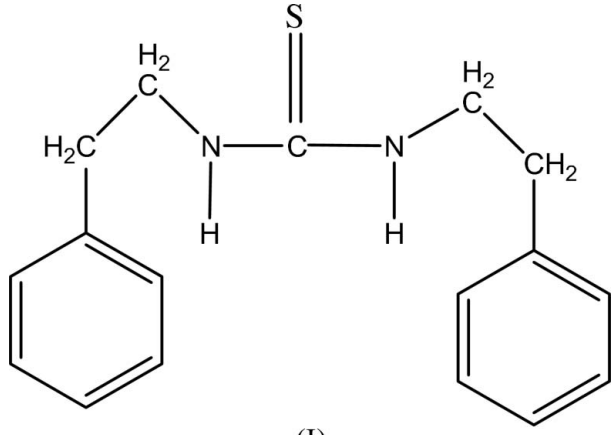
The structure of the title compound, $C_{17}H_{20}N_2S$, exhibits hydrogen bonding of the type N—H···S, resulting in chains of molecules running along the *b* axis.

## Comment

Thiourea derivatives are very useful building blocks for the synthesis of a wide range of aliphatic macromolecular and heterocyclic compounds. Benzothiazoles have been prepared from arylthioureas in the presence of bromine (Patil & Chedekel, 1984), while condensation of thiourea with halocarbonyl compounds forms 2-aminothiazoles (Bailey *et al.*, 1996). *N*-substituted and *N*,*N*′-disubstituted thiourea derivatives have potential applications due to their coordination behaviour towards transition metals (Schuster *et al.*, 1990) and their biological activity (French *et al.*, 1970). For example, aliphatic and acylthioureas are well known for their fungicidal, antiviral, pesticidal and plant-growth regulating activities (Upadhyaya & Srivastava, 1982; Wegner *et al.*, 1986). Owing to the importance of thiourea, we report the synthesis and crystal structure of *N*,*N*-bis(2-phenylethyl)thiourea, (I).




(I)

The structure (Fig. 1) is composed of independent molecules of (I) forming chains along the *b* axis *via* hydrogen bonds involving amino H atoms and S1 atoms (Table 1 and Fig. 2). The molecular dimensions are as expected (CSD, Version 5.27; Allen, 2002). Atoms S1/N1/N2/C1/C3/C10 are almost coplanar, with a maximum deviation of 0.037 (1)Å for N2 from the plane formed by these atoms; atoms C2 and C11 are displaced by 0.145 (2) and 1.308 (2) Å, respectively, out of this plane. The C4–C9 phenyl ring is almost perpendicular to the above-mentioned plane, at an angle 85.43 (5)°. The C12–C17 phenyl ring is inclined at 9.45 (7)° with respect to the

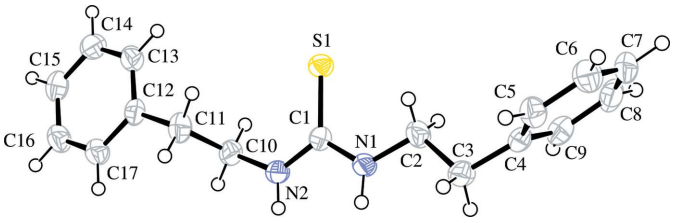



**Figure 1**
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

mean plane of atoms S1/N1/N2/C1/C3/C10. The dihedral angle between the least-squares planes of the two phenyl rings is 76.09 (6)°.

## Experimental

A solution of 2-phenylethylamine (1.0 ml, 8.26 mmol) in acetone (20 ml) was added dropwise to a solution of $CS_2$ (0.5 ml, 8.26 mmol) and $NH_4OH$ (0.6 ml, 13 mmol) in acetone (20 ml). The mixture was stirred for about 4 h at room temperature. The solution was rotary evaporated under vacuum. The crude product was then poured into acidified water (200 ml) and stirred well. The solid product (I) was separated off and recrystallized from diethyl ether (yield 78%; m.p. 356 K).

*Crystal data*

$C_{17}H_{20}N_2S$
$M_r$ = 284.41
Orthorhombic, *Pbca*
$a$ = 9.740 (2) Å
$b$ = 9.173 (2) Å
$c$ = 35.354 (9) Å
$V$ = 3158.7 (12) Å$^3$
$Z$ = 8
$D_x$ = 1.196 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.20 mm$^{-1}$
$T$ = 173 (2) K
Block, colourless
0.20 × 0.16 × 0.14 mm

*Data collection*

Nonius KappaCCD diffractometer
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
$T_{min}$ = 0.962, $T_{max}$ = 0.973
5741 measured reflections
3523 independent reflections
2385 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.037
$\theta_{max}$ = 27.6°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.100
$S$ = 1.02
3523 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.029P)^2 + 0.81P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···S1$^{i}$ | 0.88 | 2.81 | 3.563 (2) | 144 |
| N2—H2···S1$^{i}$ | 0.88 | 2.47 | 3.293 (2) | 157 |

Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, z$.

H-atoms were located in difference Fourier syntheses and were included in the refinement at geometrically idealized positions with N—H = 0.88, C—H = 0.95 and 0.99 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C,N).

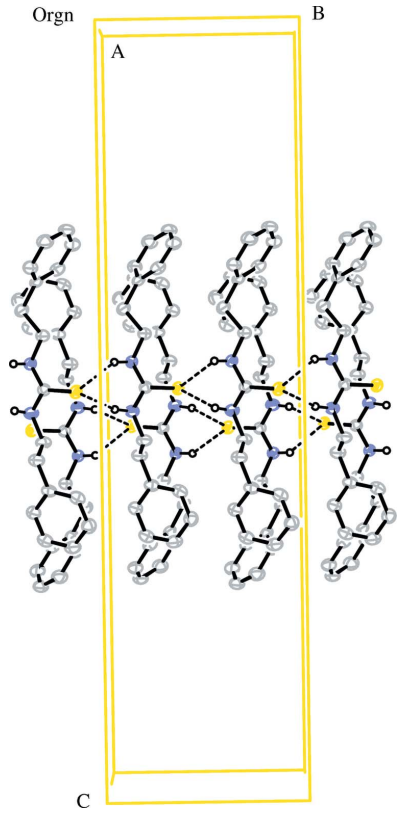



**Figure 2**
Portion of the unit-cell contents of (I), showing hydrogen-bonded chains of molecules runing along $b$ axis. Dashed lines represent hydrogen-bonding interactions. H atoms not involved in hydrogen bonding have been omitted for clarity.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SAPI91* (Fan, 1991); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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