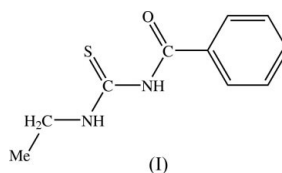


***N*-Benzoyl-*N'*-ethylthiourea****Bohari M. Yamin,\*  
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bohari@pkriscc.ukm.my**Key indicators**Single-crystal X-ray study  
 $T = 273\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$   
 $R$  factor = 0.064  
 $wR$  factor = 0.159  
Data-to-parameter ratio = 17.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title compound,  $\text{C}_{10}\text{H}_{12}\text{N}_2\text{OS}$ , the ethyl and benzoyl groups are both *cis* with respect to the S atom across the thiourea C—N bonds, in contrast with the *cis*–*trans* arrangement seen in the arylbenzoylthiourea analogues. The crystal packing is stabilized by weak intermolecular N—H···O hydrogen bonds, which form a one-dimensional polymeric chain along the *a* axis.

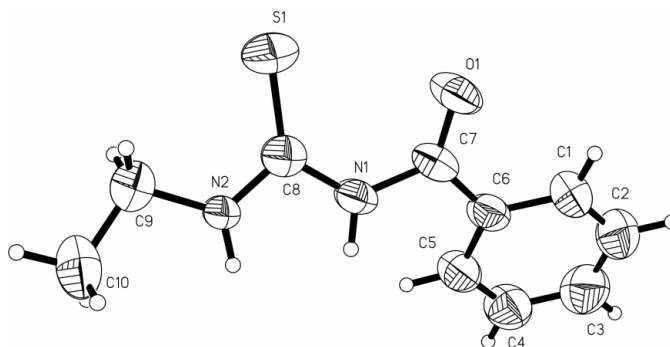
**Comment**

The structural dimensions of the title compound, (I), are in normal ranges (Allen *et al.*, 1987) and in agreement with those of other benzoylthiourea derivatives (Yamin & Yusof, 2003*a*; Shanmuga Sundara Raj *et al.*, 1999). However, the presence of an ethyl substituent at the N2 atom allows the benzoyl group to be in the *cis* position with respect to the thio group across the C8—N1 bond (Fig. 1), in contrast to the *trans* position observed in most *N*-aryl-*N'*-benzoylthioureas (Yamin & Yusof, 2003*a,b*).



The central carbonyl-thiourea moiety, including the ethyl group (S1/C8/N1/N2/C7/C8/C9/C10), is essentially planar, with a maximum deviation of 0.276 (5) Å for the C10 atom from the mean plane. The mean plane of this moiety makes an angle of 31.5 (2)° with the C1–C6 phenyl group.

In the crystal structure of (I), the molecules are linked by intermolecular N—H···O contacts (Table 2) to form a one-dimensional polymeric chain along the *a* axis (Fig. 2).

**Figure 1**

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

## Experimental

A solution of ethylamine (2.25 g, 0.05 mol) in ethanol (50 ml) was added dropwise to an equimolar amount of benzoyl isothiocyanate in ethanol (50 ml). The solution was refluxed for about 2 h and then poured into a beaker containing ice. After 2 d, white needle-shaped crystals of (I) were obtained which were suitable for X-ray analysis.

### Crystal data

$C_{10}H_{12}N_2OS$	Mo $K\alpha$ radiation
$M_r = 208.28$	Cell parameters from 1268 reflections
Orthorhombic, $Pna2_1$	$\theta = 2.8\text{--}26.9^\circ$
$a = 10.041$ (5) Å	$\mu = 0.27$ mm $^{-1}$
$b = 9.389$ (5) Å	$T = 273$ (2) K
$c = 11.450$ (6) Å	Plate, colourless
$V = 1079.5$ (9) Å $^3$	$0.45 \times 0.24 \times 0.05$ mm
$Z = 4$	
$D_x = 1.282$ Mg m $^{-3}$	

### Data collection

Bruker SMART APEX CCD area-detector diffractometer	1789 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.023$
Absorption correction: none	$\theta_{\text{max}} = 26.9^\circ$
4704 measured reflections	$h = -10 \rightarrow 12$
2171 independent reflections	$k = -11 \rightarrow 6$
	$l = -14 \rightarrow 14$

### Refinement

Refinement on $F^2$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.064$	$\Delta\rho_{\text{max}} = 0.35$ e Å $^{-3}$
$wR(F^2) = 0.159$	$\Delta\rho_{\text{min}} = -0.20$ e Å $^{-3}$
$S = 1.10$	Absolute structure: Flack (1983),
2171 reflections	936 Friedel pairs
127 parameters	Flack parameter = $-0.14$ (18)
H-atom parameters constrained	
$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2 + 0.4025P]$	
where $P = (F_o^2 + 2F_c^2)/3$	

**Table 1**

Selected geometric parameters (Å, °).

S1—C8	1.623 (4)	N1—C7	1.399 (4)
O1—C7	1.209 (4)	N2—C8	1.312 (4)
N1—C8	1.367 (5)	N2—C9	1.446 (6)
C8—N2—C9	120.4 (3)	N2—C8—N1	108.0 (3)
O1—C7—N1	121.6 (4)	N2—C8—S1	123.7 (3)

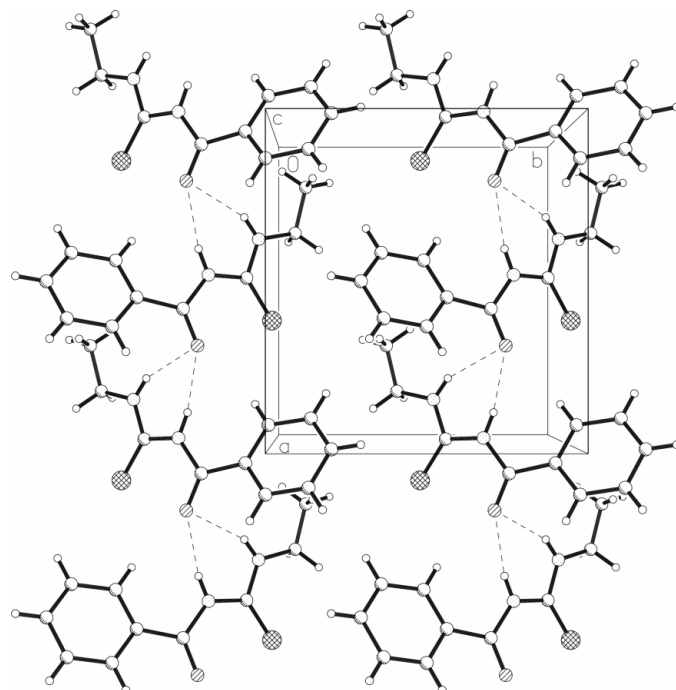
**Table 2**

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A $\cdots$ O1 $^i$	0.86	2.13	2.979 (4)	169
N2—H2A $\cdots$ O1 $^i$	0.86	2.40	3.195 (4)	154

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

After their location in a Fourier difference map, all H atoms were positioned geometrically and allowed to ride on their parent C or N



**Figure 2**

A packing diagram for (I), viewed down the  $c$  axis. Dashed lines denote the N—H $\cdots$ O intermolecular hydrogen bonds.

atoms, with C—H = 0.93–0.97 and N—H = 0.86 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5U_{\text{eq}}(\text{C})$ , or  $1.2U_{\text{eq}}(\text{N})$ .

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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