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N-(*N*-Benzoylhydrazinocarbothioyl)benzamide

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.057
wR factor = 0.133
Data-to-parameter ratio = 16.3

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

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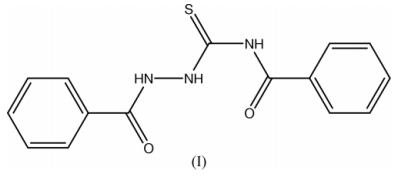
The molecular structure of the title compound, $C_{15}H_{13}N_3O_2S$, adopts a *cis–trans* configuration with respect to the position of the benzoyl and benzamide groups relative to the S atom across the thiourea C—N bonds, respectively. In the crystal structure, the molecules are linked by weak N—H···O and C—H···O interactions into linear chains parallel to the *c* axis.

Comment

The molecular structure and dimensions of the title compound, (I), are similar to those of other benzoylthiourea derivatives, such as *N*-benzoyl-*N*′-phenylthiourea (Yamin & Yusof, 2003*a*), *N*-benzoyl-*N*′-(3,4-dimethylphenyl)thiourea (Shanmuga Sundara Raj *et al.*, 1999) and *N*′-benzoyl-*N*-*p*-bromophenylthiourea (Yamin & Yusof, 2003*b*), with a *cis–trans* configuration with respect to the position of the benzamide and benzoyl groups relative to the S atom across the C8—N2 and C8—N1 bonds, respectively.



(I)

The central thiourea moiety (S1/C8/N1/N2) is planar. The benzoyl [maximum deviation at O1 of 0.348 (2) Å] and benzamide [maximum deviation at N3 of 0.306 (2) Å] fragments are essentially planar. The central thiourea moiety makes angles with the benzoyl and benzamide fragments of 15.12 (11) and 31.45 (12)°, respectively. The inclination between the benzoyl and benzamide fragments is 16.42 (14)°. There are two N—H···O and N—H···S intramolecular hydrogen bonds (Table 2). In the crystal structure, the molecules are linked by intermolecular N—H···O and C—H···O contacts (Table 2), forming linear chains parallel to the *c* axis (Fig. 2).

Experimental

A solution of benzhydrazide (1.62 g, 0.011 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 83%). Recrystallization from ethanol yielded single crystals suitable for X-ray analysis.

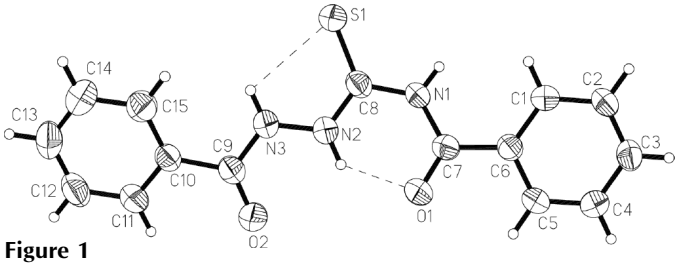


Figure 1
The molecular structure of (I), with 50% probability displacement ellipsoids. Dashed lines indicate intramolecular hydrogen bonds.

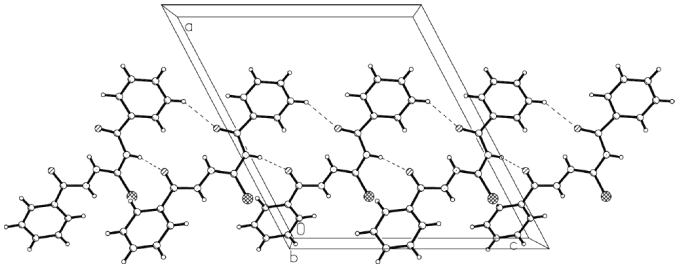


Figure 2
Packing diagram of (I), viewed down the *b* axis. The dashed lines denote the N—H···O and C—H···O intermolecular hydrogen bonds.

Crystal data

$C_{15}H_{13}N_3O_2S$
$M_r = 299.34$
Monoclinic, $P2_1/c$
$a = 14.7949\ (19)$ Å
$b = 7.7004\ (10)$ Å
$c = 13.9577\ (18)$ Å
$\beta = 117.705\ (2)^\circ$
$V = 1407.8\ (3)$ Å^3
$Z = 4$
$D_x = 1.412$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1584 reflections
$\theta = 1.6$–27.5°
$\mu = 0.24$ mm^{-1}
$T = 273\ (2)$ K
Slab, colourless
0.55 × 0.21 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.880$, $T_{max} = 0.977$
7907 measured reflections
3097 independent reflections
1925 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 27.5^\circ$
$h = -17 \rightarrow 18$
$k = -9 \rightarrow 9$
$l = -18 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.133$
$S = 1.05$
3097 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 0.1794P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C8	1.659 (3)	N1—C8	1.388 (3)
O1—C7	1.221 (3)	N2—C8	1.324 (3)
O2—C9	1.222 (3)	N2—N3	1.375 (3)
N1—C7	1.376 (3)	N3—C9	1.346 (3)
C7—N1—C8	127.3 (2)	N2—C8—N1	115.4 (2)
C9—N3—N2	119.8 (2)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.86	1.88	2.558 (3)	134
N3—H3A···S1	0.86	2.59	2.923 (2)	104
N1—H1A···O2^{i}	0.86	2.31	3.114 (3)	155
C2—H2B···O1^{i}	0.93	2.47	3.263 (4)	142

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

After their location in a difference map, all H atoms were fixed geometrically and allowed to ride on the parent C or N atoms, with C—H = 0.93 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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