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1-Benzoyl-3-(4-chlorophenyl)thiourea

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.111
Data-to-parameter ratio = 16.8

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

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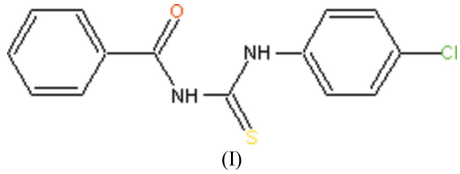
In the crystal structure of the title compound, $C_{14}H_{11}ClN_2OS$, the dihedral angle between the two aromatic ring planes is 43.93 (6)°. The crystal packing shows dimers formed by intermolecular N—H···S hydrogen bonds which are stacked along [100].

Comment

N-Substituted and *N*,*N*′-disubstituted thiourea derivatives have attracted the attention of researchers in a number of fields over the last three decades with regard to *e.g.* coordination behaviour towards transition metals (Schuster *et al.*, 1990) and biological activities (Frech *et al.*, 1970). In addition, thiourea derivatives possess antitubercular, antibacterial, antifungal, antithyroid and insecticidal properties (Madan & Taneja, 1991). The title compound, (I) (Fig. 1), is a typical *N*,*N*′-disubstituted thiourea derivative with geometric parameters common for this type of compound. Compared to *N*-benzoyl-*N*′-phenylthiourea (Yamin & Yusof, 2003) and the related 1-benzoyl-3-(3-chlorophenyl)thiourea compound (Rauf *et al.*, 2006), the different Cl substitution results in no significant effect. The dihedral angle formed between the benzene and phenyl rings is 43.93 (6)°.



(I)

The structure shows intramolecular N—H···O, as well as intermolecular N—H···S hydrogen bonds (Table 1). The latter link molecules into dimers which are stacked along [100] (Fig. 2); this is a well known structural feature for these compounds (Arslan *et al.*, 2003).

Experimental

A solution of benzoyl chloride (1.50 g, 10 mmol) in acetone (50 ml) was added dropwise to a suspension of KSCN ((1.00 g, 10 mmol) in acetone (30 ml). The reaction mixture was heated under reflux for 45 min and then cooled to room temperature. A solution of 4-chloroaniline (1.28 g, 10 mmol) in acetone (15 ml) was then added and the resulting mixture was stirred for 3 h. The reaction mixture was then poured into crushed ice and stirred well. The solid product was separated and washed with deionized water and purified by recrystallization from toluene to give fine crystals of the title compound, with an overall yield of 85%. Full spectroscopic and physical characterization will be reported elsewhere.

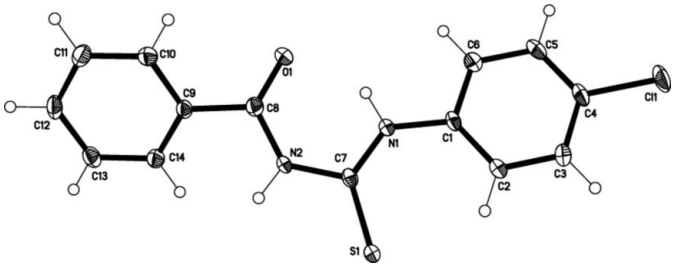


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

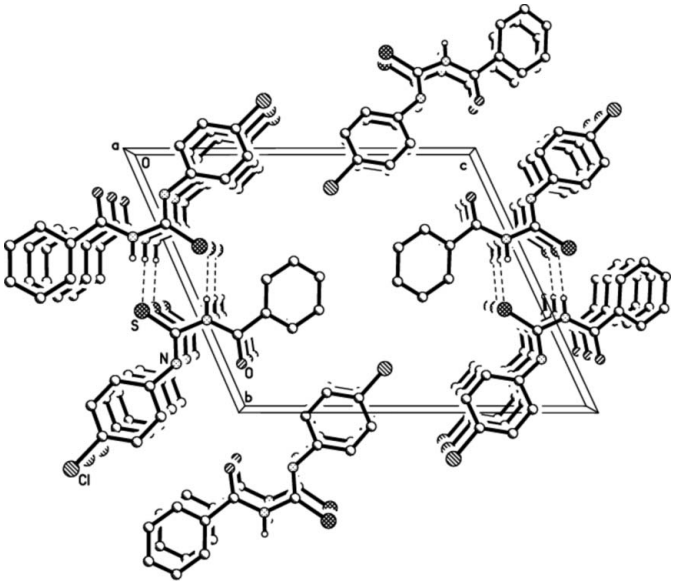


Figure 2
The crystal packing, viewed along [100], with the intermolecular hydrogen-bonds indicated by dashed lines. H atoms not involved in hydrogen bonding have been omitted.

Crystal data

$C_{14}H_{11}ClN_2OS$
$M_r = 290.76$
Triclinic, $P\overline{1}$
$a = 3.9530\ (5)$ Å
$b = 12.2293\ (14)$ Å
$c = 14.8754\ (17)$ Å
$\alpha = 65.832\ (2)^\circ$
$\beta = 89.487\ (2)^\circ$
$\gamma = 82.995\ (3)^\circ$
$V = 650.52\ (13)$ Å^3
$Z = 2$
$D_x = 1.484$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1779 reflections
$\theta = 2.8$–26.2°
$\mu = 0.45$ mm^{-1}
$T = 120\ (2)$ K
Flat needle, colorless
$0.43 \times 0.19 \times 0.06$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.832$, $T_{max} = 0.974$
5434 measured reflections
2884 independent reflections
2424 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 27.3^\circ$
$h = -5 \rightarrow 5$
$k = -15 \rightarrow 13$
$l = -19 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.111$
$S = 1.07$
2884 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2 + 0.0457P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.88	1.90	2.640 (2)	140
N2—H2B···S1^{i}	0.88	2.61	3.4686 (17)	165

Symmetry code: (i) $-x+1, -y+1, -z$.

H atoms were placed at idealized positions, N—H = 0.88 and C–H = 0.95 Å, and refined as riding on their parent C and N atoms, with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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