Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-(2-Chlorobenzoyl)-*N*-(pyrrolidin-1-yl)thiourea

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.049
wR factor = 0.107
Data-to-parameter ratio = 16.5

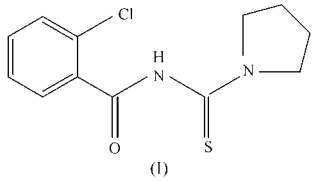
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 8 July 2003
Accepted 14 July 2003
Online 24 July 2003

In the title compound, $C_{12}H_{13}ClN_2OS$, the molecule has a twisted conformation with regard to the carbonyl and thiocarbonyl groups. In the crystal structure, hydrogen-bonded pairs of molecules are formed which stack along [100].

Comment

The title compound, (I), is another example of our newly synthesized thiourea derivatives (Arslan *et al.*, 2003*a*). Its molecular structure is closely related to that of *N*′-(4-chlorobenzoyl)-*N*,*N*-diphenylthiourea (Arslan *et al.*, 2003*b*) or anthrylcarbonyl-*N*-pyrrolidinethiourea (Bricks *et al.*, 2000). Essential bond lengths, *viz*. S1—C8 = 1.676 (3) Å, C8—N1 = 1.408 (3) Å, N1—C7 = 1.366 (3) Å and C7—O1 = 1.211 (3) Å, are similar to the corresponding bond lengths in the cited compounds. The conformation of the title molecule with respect to the thiocarbonyl and carbonyl moieties is twisted, as reflected by the C8—N1—C7—O1 and C7—N1—C8—N2 torsion angles of −4.2 (4) and 57.7 (4)°, respectively. The crystal packing is dominated by strong intermolecular N1—H1*A*···S1($-x+1$, $-y+1$, $-z+1$) hydrogen bonds, with H···S = 2.48 Å and N—H···S 151°, forming dimeric pairs of molecules that are stacked along [100]. There is a weak intramolecular interaction, C12—H12*B*···O1, with C—O 2.47 Å and an angle of 107° at H. All these values are normalized for N—H = 1.03 Å, enabling a better comparison of hydrogen-bonding geometries from different structures.



(I)

Experimental

The title compound was prepared according to the method of Arslan *et al.* (2003*a*), by converting 2-chlorobenzoyl chloride into 2-chlorobenzoyl isothiocyanate and then condensing with pyrrolidine in acetone solution at 313 K. The compound was recrystallized from ethanol.

Crystal data

$C_{12}H_{13}ClN_2OS$
M_r = 268.75
Triclinic, $P\overline{1}$
a = 7.299 (1) Å
b = 10.039 (1) Å
c = 10.096 (1) Å
α = 67.03 (1)°
β = 69.32 (1)°
γ = 88.43 (1)°
V = 631.98 (12) Å^3
Z = 2
D_x = 1.412 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 7.1–15.9°
μ = 0.45 mm^{-1}
T = 293 (2) K
Prism, colourless
0.28 × 0.25 × 0.12 mm

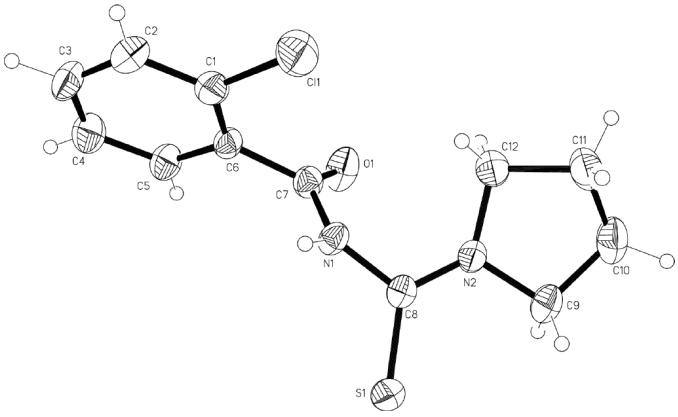


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

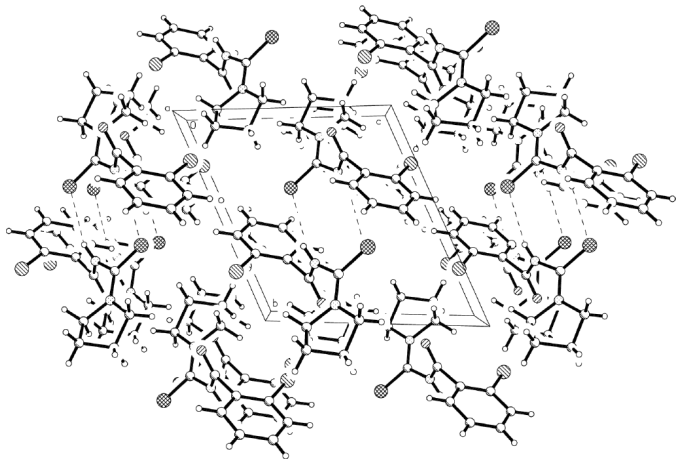


Figure 2
Packing diagram, viewed along [100]. Intermolecular hydrogen bonding is indicated by dashed lines.

Data collection

Bruker *P*4 diffractometer	$R_{int} = 0.023$
ω scans	$\theta_{max} = 26.4^\circ$
Absorption correction: ψ scan (North *et al.*, 1968)	$h = -1 \rightarrow 9$
	$k = -12 \rightarrow 12$
$T_{min} = 0.867$, $T_{max} = 0.947$	$l = -11 \rightarrow 11$
3181 measured reflections	3 standard reflections
2552 independent reflections	every 397 reflections
1692 reflections with $I > 2\sigma(I)$	intensity decay: <1%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0363P)^2 + 0.1907P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.049$	
$wR(F^2) = 0.107$	
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
2552 reflections	$\Delta\rho_{max} = 0.28$ e Å^{-3}
155 parameters	$\Delta\rho_{min} = -0.29$ e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL*97
	Extinction coefficient: 0.049 (4)

Table 1
Selected geometric parameters (Å, °).

S1—C8	1.676 (3)	N1—C8	1.408 (3)
O1—C7	1.211 (3)	N2—C8	1.312 (3)
N1—C7	1.366 (3)	C6—C7	1.502 (4)
C7—N1—C8	125.5 (2)	N2—C8—N1	116.7 (2)
O1—C7—N1	124.0 (3)	N2—C8—S1	124.0 (2)
O1—C7—C6	122.5 (3)	N1—C8—S1	119.23 (19)
N1—C7—C6	113.4 (2)		

The H atoms were introduced at calculated positions as riding atoms, with bond lengths of 0.86 (N—H), 0.93 (C—H aromatic), and 0.97 Å (CH_2). The isotropic displacement parameters, U_{iso}(H), were set equal to $1.2U_{eq}$(parent atom).

Data collection: *XSCANS* (Bruker, 1996); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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