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N-(4-Methylbenzoyl)-N'-(4-nitrophenyl)thiourea

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.128
Data-to-parameter ratio = 12.9

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

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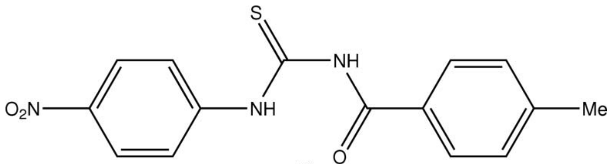
The title compound, $C_{15}H_{13}N_3O_3S$, adopts a *trans–cis* configuration of the tolyl and nitrophenyl groups, respectively, with respect to the thiono S atom across the thiourea C—N bonds. The molecule is stabilized by intermolecular hydrogen bonds, forming one-dimensional chains parallel to the *a* axis.

Comment

Some thiourea derivatives have shown promising biological activity against bacteria, fungi and cells (Baruah *et al.*, 2002). The title compound, (I), is isostructural with *N*-benzoyl-*N'*-phenylthiourea, (II) (Yamin & Yusof, 2003), and *N*-(4-chloro-3-nitrophenyl)-*N'*-(4-nitrobenzoyl)thiourea, (III) (Yusof *et al.*, 2006), but having nitro and methyl groups attached to the benzene rings (Fig. 1).



(I)

The bond lengths and angles (Table 1) are normal (Allen *et al.*, 1987) and in agreement with those in (II) and (III). The central carbonylthiourea (S1/N1/N2/C7/O1/C8), 4-methylphenyl (C1–C6/C15) and 4-nitrophenyl (C9–C14/N3/O2/O3) groups are all planar, with a maximum deviation of 0.151 (2) Å for atom O2 from the least-squares plane of the 4-nitrophenyl fragment. The central carbonylthiourea fragment makes dihedral angles of 24.67 (10) and 6.65 (10)° with the 4-methylphenyl and 4-nitrophenyl fragments, respectively. The two aryl rings are inclined to each other at an angle of 28.12 (12)°.

There is one intramolecular hydrogen bond, N2—H2*A*···O1 (Table 2), forming a pseudo-six-membered ring (O1···H2*A*—N2—C8—N1—C7—O1). In the crystal structure, the molecules are linked by intermolecular interactions, N1—H1*A*···S1 and C5—H5···O2 (symmetry codes as in Table 2), forming one-dimensional chains along the *a* axis (Fig. 2).

Experimental

To a stirred acetone solution (75 ml) of 4-methylbenzoyl chloride (2.0 g, 13 mmol) and ammonium thiocyanate (0.98 g, 13 mmol), a solution of 4-nitrophenylamine (1.79 g, 13 mmol) in acetone (30 ml) was added dropwise. The resulting mixture was refluxed for 1 h. The resulting solution was poured into a beaker containing some ice blocks. The light-yellow precipitate was filtered off, washed with distilled water and cold ethanol, and then dried under vacuum. Good quality crystals were obtained by recrystallization from chloroform (yield 76%, 2.53 g; m.p. 460.29–462.93 K).

Crystal data

$C_{15}H_{13}N_3O_3S$
$M_r = 315.34$
Monoclinic, $P2_1/c$
$a = 12.237$ (3) Å
$b = 6.3181$ (15) Å
$c = 19.362$ (5) Å
$\beta = 101.976$ (4)°
$V = 1464.4$ (6) Å^3
$Z = 4$
$D_x = 1.430$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.24$ mm^{-1}
$T = 293$ (2) K
Slab, light yellow
0.40 × 0.31 × 0.11 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\rm min} = 0.911$, $T_{\rm max} = 0.974$
7216 measured reflections
2572 independent reflections
2004 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.027$
$\theta_{\rm max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.128$
$S = 1.00$
2572 reflections
200 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0714P)^2 + 0.407P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.19$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C8	1.649 (2)	N1—C8	1.392 (3)
N1—C7	1.383 (3)	N2—C8	1.339 (3)
C7—N1—C8	129.90 (19)	N2—C8—S1	128.49 (18)
N2—C8—N1	114.04 (19)	N1—C8—S1	117.48 (16)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1	0.86	1.91	2.640 (3)	142
N1—H1*A*···S1$^{\rm i}$	0.86	2.75	3.490 (2)	145
C5—H5···O2$^{\rm ii}$	0.93	2.57	3.474 (4)	165

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x+1, -y+2, -z$.

After their location in a difference map, all H atoms were positioned geometrically and allowed to ride on their parent C or N atoms, with C—H = 0.93–0.96Å, N—H = 0.86Å and $U_{\rm iso}$(H)= 1.2 (CH_2 and NH) or 1.5 (CH_3) times $U_{\rm eq}$(C,N).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

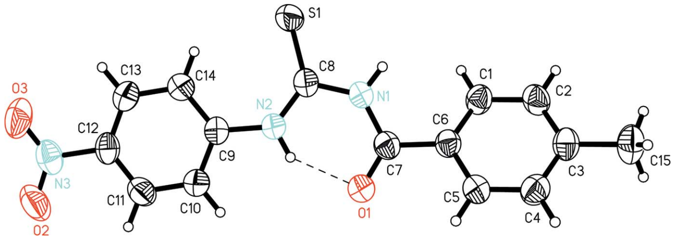


Figure 1
Fig. 1. The molecular structure of the title compound, (I), shown with 50% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

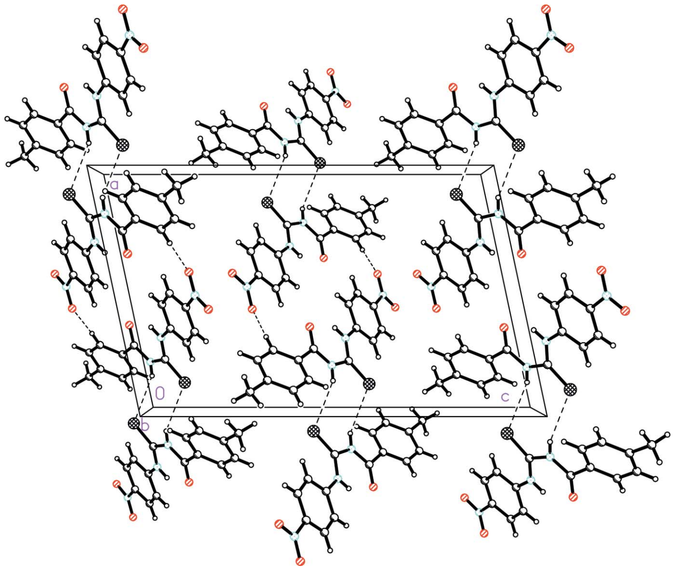


Figure 2
Packing diagram of (I), viewed down the *b* axis. Dashed lines denote the N—H···S and C—H···O hydrogen bonds.

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