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1-[(Phenyl)(*p*-tolylimino)methyl]-3-(*o*-tolyl)thiourea

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In the crystal structure of the title compound, $C_{22}H_{21}N_3S$, intermolecular N—H···S hydrogen bonds link the molecules into hydrogen-bonded dimers. There is an intramolecular N—H···N hydrogen bond.

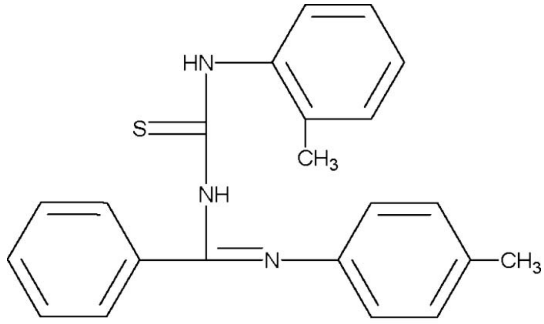
Key indicators

Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.112
Data-to-parameter ratio = 18.2

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

Comment

Thiourea derivatives are very important intermediates in organic syntheses, and have been widely utilized in medicinal chemistry (Smith *et al.*, 1996) and photochemistry (Dittami *et al.*, 1996; Jayanthi *et al.*, 1997). In order to study their photochemical behavior, we synthesized a series of new thiourea derivatives (Xing & Zhao, 2006*a*,*b*). Here we report the crystal structure of the title compound, (I). An intramolecular hydrogen bond (Table 1 and Fig. 1) appears to influence the conformation of the molecule. The resulting six-membered ring (C9/N2/C1/N1/N3/H1) is essentially planar, with an r.m.s. deviation for the fitted atoms of 0.070 Å. In the crystal structure, pairs of molecules form centrosymmetric dimers *via* intermolecular N—H···S hydrogen bonds (Table 1 and Fig. 2).



(I)

Experimental

The title compound was prepared according to a literature procedure (van den Nieuwendijk *et al.*, 2004). Single crystals of the title compound suitable for X-ray analysis were obtained from acetonitrile solution.

Crystal data

$C_{22}H_{21}N_3S$
M_r = 359.48
Triclinic, $P\overline{1}$
a = 10.085 (3) Å
b = 10.288 (3) Å
c = 10.301 (3) Å
α = 76.521 (13)°
β = 65.832 (11)°
γ = 88.294 (16)°
V = 945.6 (5) Å^3
Z = 2
D_x = 1.263 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 113 (2) K
Block, colorless
0.24 × 0.16 × 0.14 mm

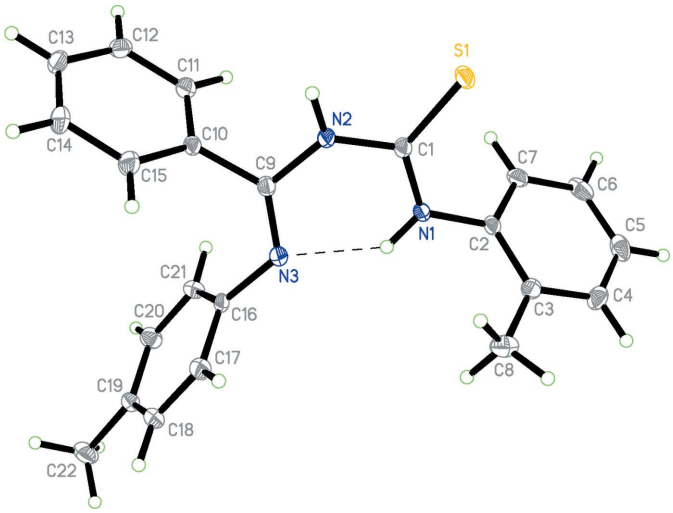


Figure 1
The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radii. The intramolecular hydrogen bond is shown as a dashed line.

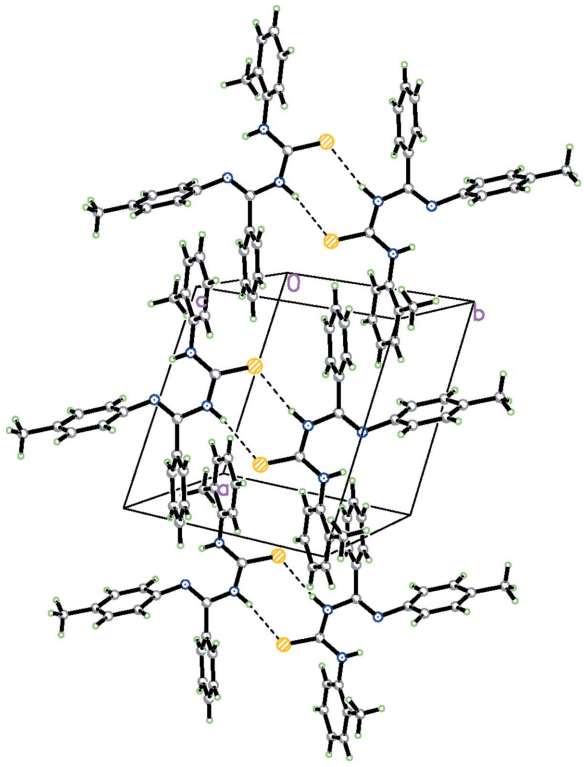


Figure 2
The packing of (I), showing the intermolecular hydrogen bonds as dashed lines.

Data collection

Rigaku Saturn diffractometer
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.958, T_{max} = 0.975
11995 measured reflections
4500 independent reflections
3237 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 27.9°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.112
S = 1.04
4500 reflections
247 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0789P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.029 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···S1^{i}	0.888 (17)	2.458 (17)	3.3314 (16)	167.9 (14)
N1—H1···N3	0.895 (16)	1.991 (16)	2.7214 (18)	137.8 (14)

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

All H atoms were initially located in a difference Fourier map. The C—H atoms were then constrained to an ideal geometry, with methyl C—H distances of 0.98 Å and aromatic C—H distances of 0.95 Å, and with U_{iso}(H) = 1.2U_{eq}(C). The amino H atoms were refined freely.

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *CrystalStructure*.

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