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1,3-Di-*o*-tolylthiourea

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Key indicators

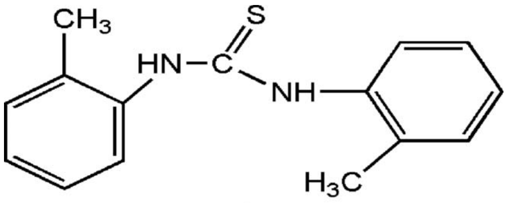
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.105
Data-to-parameter ratio = 15.0

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

The two *o*-tolyl groups in the title compound, $C_{15}H_{16}N_2S$, are *trans* with respect to the thiourea unit. The asymmetric unit consists of two molecules linked by N—H···S hydrogen bonds into dimers.

Comment

The biological properties of thiourea complexes are well documented and thiourea derivatives have been successfully screened for various biological activities (Frech *et al.*, 1970). Thiourea derivatives are also useful ligands to a number of metals (König *et al.*, 1984; Schuster *et al.*, 1990). The molecular structure of the title thiourea derivative, (I), is reported here (Fig. 1).



(I)

There are two molecules in the asymmetric unit. The short C—S distances in (I) [1.6938 (16) and 1.6927 (16) Å] clearly shows double-bond character. For one molecule, the dihedral angles between the thiourea bridge and the C17- and C114-tolyl rings are 88.79 (8) and 61.05 (8)°, respectively, with the angle between the tolyl ring planes being 58.98 (8)°. The corresponding values for the second molecule are 87.61 (8), 79.61 (8) and 59.04 (8)°, respectively.

The two tolyl rings are mutually *trans* with respect to the N11—C115 or N21—C215 bonds of the thiourea units. This configuration favours dimer formation between the molecules (Ramnathan *et al.*, 1996) and, in this case, intermolecular N—H···S hydrogen bonds link the molecules into dimers (Fig. 2).

Experimental

A solution of *o*-toluidine (1.1 ml, 10 mmol) in acetone (20 ml) was added dropwise to a solution of CS_2 (0.90 ml, 10 mmol) and NH_3 (0.60 ml, 15 mmol) in acetone (50 ml). The mixture was stirred for about 4 h at room temperature and was then rotary-evaporated under vacuum. The crude product was added to 10% HCl (200 ml) and stirred well. The solid product was separated off and recrystallized from diethyl ether. The yield was 78%.

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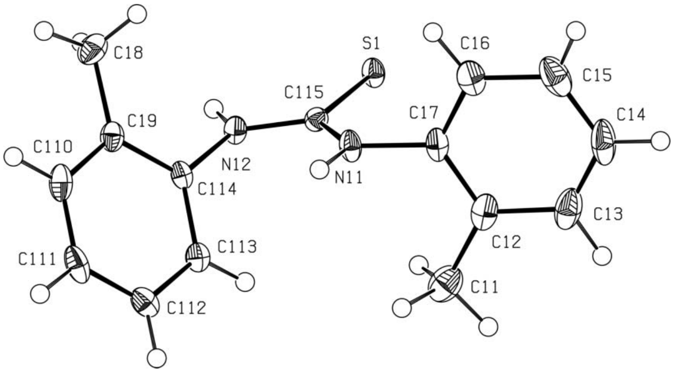

Figure 1
The structure of molecule 1 of the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

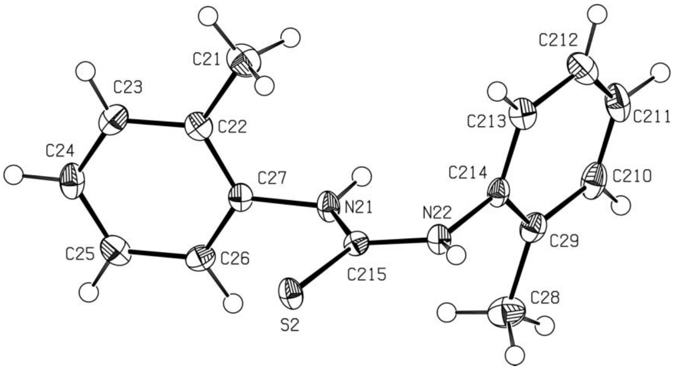

Figure 2
The structure of molecule 2 of the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

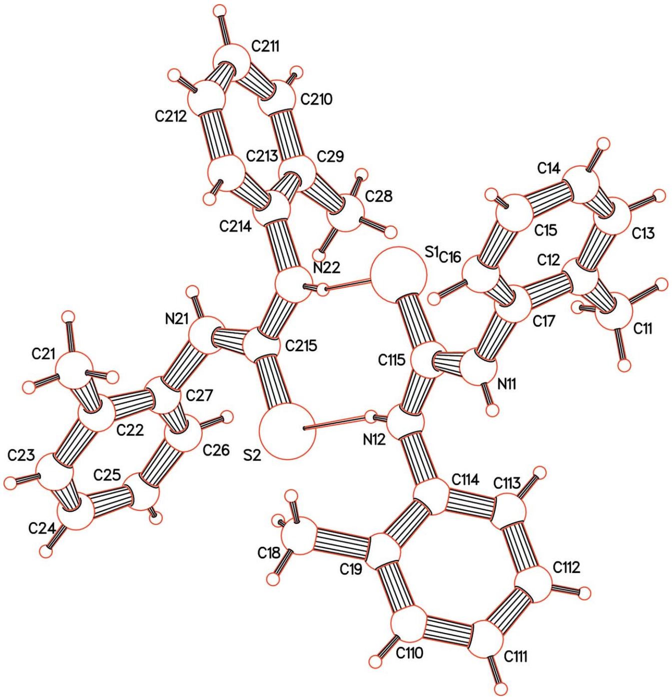

Figure 3
A perspective *PLUTO* (Meetsma, 2006) drawing of the dimer formed by N—H···S hydrogen bonds (narrow lines).

Crystal data

$C_{15}H_{16}N_2S$
$M_r = 256.37$
Monoclinic, $P2_1/n$
$a = 12.3960$ (9) Å
$b = 9.5652$ (7) Å
$c = 23.163$ (2) Å
$\beta = 92.266$ (1)°
$V = 2744.3$ (4) Å^3
$Z = 8$
$D_x = 1.241$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.22$ mm^{-1}
$T = 100$ (1) K
Block, colourless
0.49 × 0.23 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.886$, $T_{\max} = 0.966$
22738 measured reflections
6776 independent reflections
5577 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.034$
$\theta_{\max} = 28.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.105$
$S = 1.05$
6776 reflections
453 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 1.5124P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.37$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N12—H122···S2	0.87 (2)	2.49 (2)	3.3408 (14)	165.4 (18)
N22—H222···S1	0.87 (2)	2.43 (2)	3.2794 (14)	166.9 (17)

All H atoms were located in a difference Fourier map and were refined with isotropic displacement parameters [C—H = 0.92 (3)–1.03 (3) Å and N—H = 0.83 (2)–0.84 (2) Å].

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLUTO* (Meetsma, 2006) and *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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