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1-(3,5-Dimethylphenyl)-3-phenylthiourea

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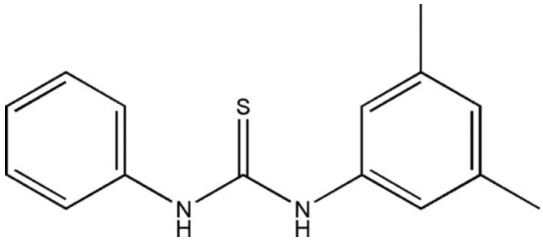
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.135; data-to-parameter ratio = 18.3.

The title compound, $C_{15}H_{16}N_2S$, was prepared by the reaction of 3,5-dimethylphenylamine with 1-isothiocyanatobenzene. In the molecule, all bond lengths and angles are within normal ranges. The dihedral angle between the two aromatic rings is 48.77 (1)°. The crystal packing is stabilized by van der Waals forces.

Related literature

For related literature, see: Antholine & Taketa (1982); Ji *et al.* (2002); Mao *et al.* (1999); Shen *et al.* (1998).



Experimental

Crystal data

$C_{15}H_{16}N_2S$
M_r = 256.36
Triclinic, $P\overline{1}$
a = 8.3740 (17) Å
b = 9.1870 (18) Å
c = 9.889 (2) Å
α = 107.57 (3)°
β = 98.57 (3)°
γ = 94.42 (3)°
V = 711.2 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 293 (2) K
0.20 × 0.18 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
3177 measured reflections
2975 independent reflections
2373 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.135
S = 1.05
2975 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2224).

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supplementary materials

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1-(3,5-Dimethylphenyl)-3-phenylthiourea

F.-F. Jian, R.-R. Zhuang, H.-L. Xiao and P.-S. Zhao

Comment

Thiosemicarbazides are able to form complexes with biological activities (Shen *et al.*, 1998). Thiourea derivatives have been successful screened for various biological activities (Antholine & Taketa,1982), and some of them have shown promising anti-HIV properties (Mao *et al.*, 1999) . The title compound was synthesized as part of our study of these ligands. Here we report the crystal structure of (I).

In (I) (Fig. 1),the bond lengths and angles are usual for this type of compound (Ji *et al.*, 2002). The mean planes p1(S1,N1,N2,C8,C9,C10) and p2 (N1,C1,C2,C3,C4,C5,C6,C7) make a dihedral angle of 59.69 (1)°. The dihedral angles formed by phenyl ring (C3,C4,C5,C6,C7,C8) and phenyl ring (C10,C11,C12,C13,C14,C15) with p1 are 59.82 (2)and 52.72 (2)° respectively. The dihedral angles between the benzene rings is 48.77 (1)°. The crystal packing is stabilized by van der Waals forces.

Experimental

A mixture of 3,5-Dimethyl-phenylamine (0.02 mol) and 1-isothiocyanatobenzeneat (0.02 mol) was stirred in refluxing ethanol (30 ml) for 0.5 h to afford the title compound (4.35 g, yield 85%). Single crystals suitable for X-ray measurementswere obtained by recrystallization from ethanol at room temperature.

Refinement

H atoms were fixed geometrically and allowed to ride on their parent atoms, with N—H and C—H distances of 0.86 and 0.93–0.96 Å, respectively, and with U_{iso}=1.2–1.5U_{eq} of the parent atoms.

Figures

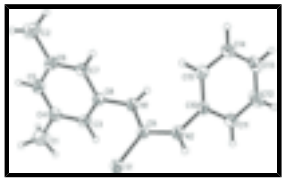

Fig. 1. The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

1-(3,5-Dimethylphenyl)-3-phenylthiourea

Crystal data

$C_{15}H_{16}N_2S$	$Z = 2$
$M_r = 256.36$	$F_{000} = 272$

Triclinic, $P\bar{1}$	D_x = 1.197 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.3740 (17) Å	Cell parameters from 25 reflections
b = 9.1870 (18) Å	θ = 4–14º
c = 9.889 (2) Å	μ = 0.21 mm^{-1}
α = 107.57 (3)º	T = 293 (2) K
β = 98.57 (3)º	Block, colourless
γ = 94.42 (3)º	0.20 × 0.18 × 0.15 mm
V = 711.2 (2) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.014
Radiation source: fine-focus sealed tube	θ_{max} = 27.0º
Monochromator: graphite	θ_{min} = 2.2º
T = 293(2) K	h = 0→9
ω scans	k = −10→10
Absorption correction: none	l = −11→11
3177 measured reflections	3 standard reflections
2975 independent reflections	every 100 reflections
2373 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0792P)^2 + 0.1571P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.043	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.135	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
S = 1.05	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
2975 reflections	Extinction correction: none
163 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.38703 (6)	0.61876 (6)	0.35631 (5)	0.05568 (19)
N1	0.17597 (19)	0.76385 (18)	0.51155 (16)	0.0481 (4)
H1A	0.1340	0.7829	0.5883	0.058*
N2	0.31741 (19)	0.59706 (19)	0.60148 (16)	0.0499 (4)
H2A	0.3850	0.5304	0.5884	0.060*
C1	0.2911 (3)	1.1300 (3)	0.2466 (3)	0.0826 (8)
H1B	0.3984	1.1334	0.2987	0.124*
H1C	0.2584	1.2312	0.2728	0.124*
H1D	0.2915	1.0943	0.1449	0.124*
C2	−0.2810 (3)	0.8645 (4)	0.1871 (3)	0.0815 (8)
H2B	−0.3012	0.9263	0.1251	0.122*
H2C	−0.3452	0.8911	0.2617	0.122*
H2D	−0.3101	0.7576	0.1318	0.122*
C3	0.2287 (2)	0.9438 (2)	0.3790 (2)	0.0477 (4)
H3A	0.3381	0.9609	0.4218	0.057*
C4	0.1728 (2)	1.0214 (2)	0.2835 (2)	0.0513 (5)
C5	0.0072 (2)	0.9943 (2)	0.2225 (2)	0.0507 (5)
H5A	−0.0310	1.0453	0.1584	0.061*
C6	−0.1017 (2)	0.8935 (2)	0.2548 (2)	0.0492 (4)
C7	−0.0428 (2)	0.8165 (2)	0.34959 (19)	0.0452 (4)
H7A	−0.1138	0.7483	0.3724	0.054*
C8	0.1213 (2)	0.84127 (19)	0.40996 (18)	0.0419 (4)
C9	0.2877 (2)	0.6635 (2)	0.49727 (18)	0.0417 (4)
C10	0.2511 (2)	0.6231 (2)	0.73090 (18)	0.0418 (4)
C11	0.3591 (3)	0.6609 (3)	0.8603 (2)	0.0635 (6)
H11A	0.4707	0.6749	0.8619	0.076*
C12	0.3007 (3)	0.6779 (3)	0.9874 (2)	0.0723 (7)
H12A	0.3736	0.7021	1.0740	0.087*
C13	0.1356 (3)	0.6592 (2)	0.9868 (2)	0.0579 (5)
H13A	0.0973	0.6729	1.0728	0.069*
C14	0.0281 (2)	0.6203 (2)	0.8582 (2)	0.0531 (5)
H14A	−0.0833	0.6064	0.8572	0.064*
C15	0.0849 (2)	0.6016 (2)	0.7296 (2)	0.0461 (4)
H15A	0.0117	0.5747	0.6429	0.055*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0619 (3)	0.0785 (4)	0.0472 (3)	0.0398 (3)	0.0248 (2)	0.0356 (2)

N1	0.0564 (9)	0.0570 (9)	0.0464 (8)	0.0294 (7)	0.0211 (7)	0.0282 (7)
N2	0.0534 (9)	0.0676 (10)	0.0466 (8)	0.0331 (8)	0.0205 (7)	0.0327 (7)
C1	0.0739 (16)	0.0851 (17)	0.114 (2)	0.0088 (13)	0.0233 (15)	0.0667 (17)
C2	0.0535 (13)	0.102 (2)	0.0914 (19)	0.0119 (13)	−0.0059 (12)	0.0430 (16)
C3	0.0422 (9)	0.0523 (10)	0.0547 (10)	0.0127 (8)	0.0092 (8)	0.0241 (8)
C4	0.0566 (11)	0.0489 (10)	0.0591 (11)	0.0140 (8)	0.0172 (9)	0.0280 (9)
C5	0.0606 (12)	0.0508 (10)	0.0497 (10)	0.0219 (9)	0.0094 (8)	0.0259 (8)
C6	0.0462 (10)	0.0501 (10)	0.0525 (10)	0.0155 (8)	0.0061 (8)	0.0169 (8)
C7	0.0464 (10)	0.0440 (9)	0.0508 (10)	0.0130 (7)	0.0136 (8)	0.0194 (8)
C8	0.0473 (10)	0.0430 (9)	0.0436 (9)	0.0193 (7)	0.0144 (7)	0.0193 (7)
C9	0.0412 (9)	0.0495 (9)	0.0404 (8)	0.0167 (7)	0.0095 (7)	0.0196 (7)
C10	0.0472 (9)	0.0451 (9)	0.0417 (9)	0.0138 (7)	0.0131 (7)	0.0220 (7)
C11	0.0443 (10)	0.1004 (17)	0.0518 (11)	0.0002 (10)	0.0069 (8)	0.0360 (11)
C12	0.0680 (14)	0.1048 (19)	0.0416 (11)	−0.0103 (13)	0.0039 (10)	0.0279 (11)
C13	0.0745 (14)	0.0600 (12)	0.0488 (11)	0.0094 (10)	0.0270 (10)	0.0236 (9)
C14	0.0512 (11)	0.0538 (11)	0.0683 (13)	0.0142 (8)	0.0252 (9)	0.0313 (9)
C15	0.0456 (10)	0.0492 (10)	0.0482 (10)	0.0111 (7)	0.0084 (7)	0.0212 (8)

Geometric parameters (Å, °)

S1—C9	1.6897 (17)	C4—C5	1.398 (3)
N1—C9	1.356 (2)	C5—C6	1.388 (3)
N1—C8	1.439 (2)	C5—H5A	0.9300
N1—H1A	0.8600	C6—C7	1.393 (2)
N2—C9	1.350 (2)	C7—C8	1.386 (3)
N2—C10	1.432 (2)	C7—H7A	0.9300
N2—H2A	0.8600	C10—C11	1.383 (3)
C1—C4	1.512 (3)	C10—C15	1.388 (3)
C1—H1B	0.9600	C11—C12	1.386 (3)
C1—H1C	0.9600	C11—H11A	0.9300
C1—H1D	0.9600	C12—C13	1.378 (3)
C2—C6	1.518 (3)	C12—H12A	0.9300
C2—H2B	0.9600	C13—C14	1.375 (3)
C2—H2C	0.9600	C13—H13A	0.9300
C2—H2D	0.9600	C14—C15	1.390 (3)
C3—C8	1.384 (3)	C14—H14A	0.9300
C3—C4	1.395 (2)	C15—H15A	0.9300
C3—H3A	0.9300		
C9—N1—C8	125.94 (14)	C7—C6—C2	120.04 (19)
C9—N1—H1A	117.0	C8—C7—C6	120.14 (17)
C8—N1—H1A	117.0	C8—C7—H7A	119.9
C9—N2—C10	128.50 (14)	C6—C7—H7A	119.9
C9—N2—H2A	115.8	C3—C8—C7	120.93 (16)
C10—N2—H2A	115.8	C3—C8—N1	120.63 (16)
C4—C1—H1B	109.5	C7—C8—N1	118.36 (16)
C4—C1—H1C	109.5	N2—C9—N1	117.07 (15)
H1B—C1—H1C	109.5	N2—C9—S1	119.88 (12)
C4—C1—H1D	109.5	N1—C9—S1	123.04 (13)
H1B—C1—H1D	109.5	C11—C10—C15	119.58 (17)

H1C—C1—H1D	109.5	C11—C10—N2	117.76 (16)
C6—C2—H2B	109.5	C15—C10—N2	122.50 (16)
C6—C2—H2C	109.5	C10—C11—C12	119.82 (19)
H2B—C2—H2C	109.5	C10—C11—H11A	120.1
C6—C2—H2D	109.5	C12—C11—H11A	120.1
H2B—C2—H2D	109.5	C13—C12—C11	120.8 (2)
H2C—C2—H2D	109.5	C13—C12—H12A	119.6
C8—C3—C4	119.93 (17)	C11—C12—H12A	119.6
C8—C3—H3A	120.0	C14—C13—C12	119.49 (18)
C4—C3—H3A	120.0	C14—C13—H13A	120.3
C3—C4—C5	118.50 (17)	C12—C13—H13A	120.3
C3—C4—C1	119.87 (19)	C13—C14—C15	120.41 (18)
C5—C4—C1	121.63 (18)	C13—C14—H14A	119.8
C6—C5—C4	121.90 (16)	C15—C14—H14A	119.8
C6—C5—H5A	119.1	C10—C15—C14	119.91 (17)
C4—C5—H5A	119.1	C10—C15—H15A	120.0
C5—C6—C7	118.59 (17)	C14—C15—H15A	120.0
C5—C6—C2	121.36 (18)		
C8—C3—C4—C5	0.8 (3)	C10—N2—C9—N1	−3.0 (3)
C8—C3—C4—C1	−178.3 (2)	C10—N2—C9—S1	177.62 (15)
C3—C4—C5—C6	0.2 (3)	C8—N1—C9—N2	−176.96 (17)
C1—C4—C5—C6	179.3 (2)	C8—N1—C9—S1	2.4 (3)
C4—C5—C6—C7	−0.7 (3)	C9—N2—C10—C11	−126.3 (2)
C4—C5—C6—C2	−179.7 (2)	C9—N2—C10—C15	58.1 (3)
C5—C6—C7—C8	0.2 (3)	C15—C10—C11—C12	−0.4 (3)
C2—C6—C7—C8	179.1 (2)	N2—C10—C11—C12	−176.1 (2)
C4—C3—C8—C7	−1.3 (3)	C10—C11—C12—C13	−0.8 (4)
C4—C3—C8—N1	−178.10 (17)	C11—C12—C13—C14	1.3 (4)
C6—C7—C8—C3	0.9 (3)	C12—C13—C14—C15	−0.8 (3)
C6—C7—C8—N1	177.69 (16)	C11—C10—C15—C14	0.9 (3)
C9—N1—C8—C3	−63.1 (3)	N2—C10—C15—C14	176.39 (16)
C9—N1—C8—C7	120.0 (2)	C13—C14—C15—C10	−0.4 (3)

Fig. 1