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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.040
 wR factor = 0.114
Data-to-parameter ratio = 14.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*N*-(4-Methoxybenzoyl)-*N'*-(4-methylphenyl)thiourea

The molecular structure of the title compound, $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_2\text{S}$, adopts a *trans-cis* configuration with respect to the position of the 4-methoxybenzoyl and 4-methylphenyl groups relative to the S atom across the thiourea C—N bonds. The 4-methylphenyl fragment is inclined to the 4-methoxybenzoyl group by $70.62(9)^\circ$. The molecule is stabilized by intermolecular N—H \cdots S interactions, forming a dimer.

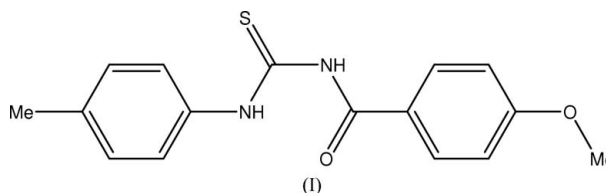
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Comment

The title compound, (I), is isomeric and isostructural with *N*-(4-methoxybenzoyl)-*N'*-*o*-tolylthiourea (Yusof & Yamin, 2004). The *trans-cis* configuration with respect to the position of the 4-methoxybenzoyl and 4-methylphenyl groups relative to the S atom across the thiourea C8—N1 and C8—N2 bonds, respectively, is maintained.



The carbonylthiourea (S1/N1/N2/C7/O1/C8), 4-methoxybenzoyl (C1—C6/O2/C15) and 4-methylphenyl (C9—C14/C16) groups are each planar. The maximum deviation is 0.035 (1) Å for atom N1 from the mean plane in the carbonylthiourea group. The dihedral angles between the carbonylthiourea group and the 4-methoxyphenyl and 4-methylphenyl fragments of $27.33(7)^\circ$ and $43.37(8)^\circ$, respectively, are larger than those in *N*-(4-methoxybenzoyl)-*N'*-*o*-tolylthiourea [$15.58(7)^\circ$ and $22.76(8)^\circ$, respectively]. The inclination between the aryl fragments of $70.62(9)^\circ$ is larger than that of $7.58(9)^\circ$ in *N*-(4-methoxybenzoyl)-*N'*-*o*-tolylthiourea.

There are two intramolecular hydrogen bonds, *viz.* N2—H2A \cdots O1 and C14—H14 \cdots S1 (Table 2), and as a result, two pseudo-six-membered rings (C8—N2—C9—C14—H14 \cdots S1

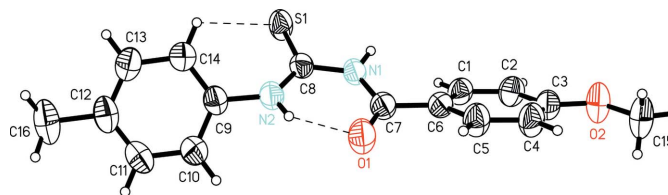


Figure 1

The molecular structure of (I), with 50% probability displacement ellipsoids. The dashed lines indicate the intramolecular hydrogen-bond contacts.

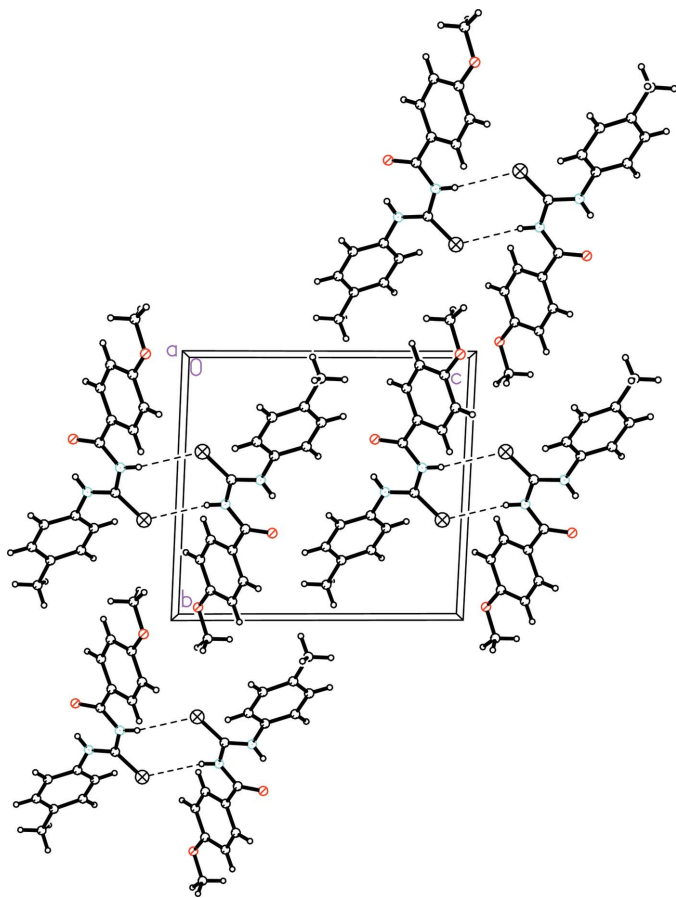


Figure 2
Packing diagram of compound (I), viewed down the *a* axis. The dashed lines denote N—H···S hydrogen bonds, which form a dimer.

and C7—N1—C8—N2—H2A···O1) are formed. In the crystal structure, molecules are linked by intermolecular interactions, N1—H1A···S1ⁱ [symmetry code: (i) 1 - *x*, 1 - *y*, 2 - *z*], forming a centrosymmetric dimer.

Experimental

To a stirred acetone solution (75 ml) of anisoyl chloride (2.5 g, 20 mmol) and ammonium thiocyanate (2.1 ml, 20 mmol), *p*-toluidine (2.8 ml, 20 mmol) was added dropwise. The mixture was refluxed for 3 h. The resulting solution was poured into a beaker containing ice cubes. The white precipitate was filtered off and washed with distilled water and cold ethanol, and then dried in a vacuum. Good quality single crystals were obtained by recrystallization from dimethyl sulfoxide.

Crystal data

C₁₆H₁₆N₂O₂S
M_r = 300.37
 Triclinic, *P*1̄
a = 5.3676 (9) Å
b = 11.4763 (19) Å
c = 12.447 (2) Å
 α = 92.505 (3)°
 β = 91.692 (3)°
 γ = 94.138 (3)°
V = 763.6 (2) Å³

Z = 2
D_x = 1.306 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 951 reflections
 θ = 1.6–25.5°
 μ = 0.22 mm⁻¹
T = 293 (2) K
 Block, colourless
 0.45 × 0.39 × 0.30 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.90, *T_{max}* = 0.93
 7554 measured reflections

2827 independent reflections
 2492 reflections with *I* > 2σ(*I*)
R_{int} = 0.016
 θ_{\max} = 25.5°
h = -6 → 6
k = -13 → 13
l = -15 → 15

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.040
wR (*F*²) = 0.114
S = 1.08
 2827 reflections
 192 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0606P)^2 + 0.149P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.21 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.16 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

S1—C8	1.6640 (16)	N1—C8	1.385 (2)
O1—C7	1.225 (2)	N2—C8	1.328 (2)
O2—C3	1.353 (2)	N2—C9	1.427 (2)
N1—C7	1.376 (2)		
N2—C8—N1	116.22 (14)	N1—C8—S1	117.81 (12)
N2—C8—S1	125.97 (12)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N2—H2A···O1	0.86	1.94	2.640 (2)	138
C14—H14···S1	0.93	2.79	3.1980 (19)	108
N1—H1A···S1 ⁱ	0.86	2.72	3.5305 (16)	158

Symmetry code: (i) -*x* + 1, -*y* + 1, -*z* + 2.

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 = 0.93–0.96 Å and N—H = 0.86 Å, and *U*_{iso}(H) = 1.2*U*_{eq}(C,N) for CH₂ and NH, and 1.5*U*_{eq}(C) for CH₃.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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