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N-(4-Methoxyphenyl)-*N*′-(2-methylbenzoyl)-thiourea

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In the title molecule, $C_{16}H_{16}N_2O_2S$, all bond lengths and angles show normal values. The mean plane of the carbonylthiourea fragment makes dihedral angles of 58.56 (18) and 48.89 (16)° with the mean planes of the 2-methylbenzoyl and 4-methoxyphenyl groups, respectively. In the crystal structure, weak intermolecular N—H···O and N—H···S hydrogen bonds link the molecules into ribbons running in the [110] direction.

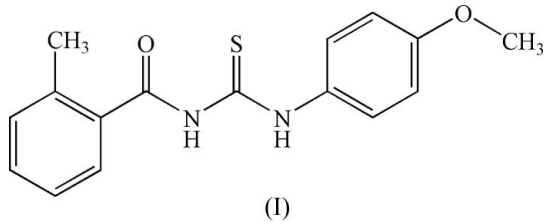
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.070
wR factor = 0.208
Data-to-parameter ratio = 15.6

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

Comment

Aroylthiourea derivatives have attracted much attention due to their biological activities (Du *et al.*, 2002; Sun *et al.*, 2006; Xu *et al.*, 2003) and coordination abilities (Koch, 2001). The title compound, (I), belongs to the family of aroylthiourea derivatives. We present here its crystal structure.



(I)

In (I) (Fig. 1), all bond lengths and angles show normal values (Allen *et al.*, 1987), which are in good agreement with those observed in related compounds (Cao *et al.*, 1996; Yamin & Yusof, 2003). An intramolecular N2—H2*A*···O1 hydrogen bond (Table 1) influences the molecular geometry. The mean planes of the carbonylthiourea (O1/C8/N1/C9/S1/N2, *A*), 2-methylbenzoyl (C1–C7, *B*) and 4-methoxylphenyl (C10–C15/O2/C16, *C*) groups make the following dihedral angles: *A*/*B* 58.56 (18)°, *A*/*C* 48.89 (16)° and *B*/*C* 9.73 (17)°.

In the crystal structure (Fig. 2), weak intermolecular N—H···O and N—H···S hydrogen bonds (Table 1) link the molecules into ribbons running in the [110] direction.

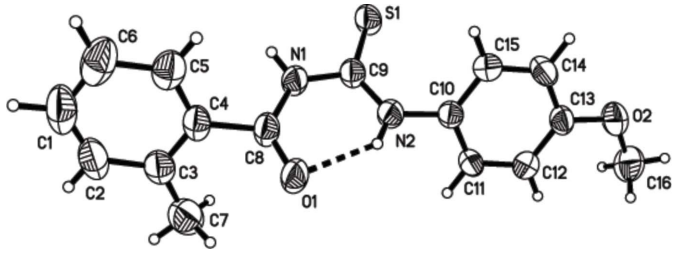


Figure 1
The molecular structure of (I), showing the atom-labelling scheme and displacement ellipsoids drawn at the 50% probability level. The dashed line indicates the intramolecular hydrogen bond.

Experimental

The title compound was prepared according to the literature method of Feng *et al.* (1992). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a DMF solution at 293 K.

Crystal data

$C_{16}H_{16}N_2O_2S$
M_r = 300.37
Monoclinic, $P2_1/n$
a = 7.6910 (15) Å
b = 7.6740 (15) Å
c = 25.619 (5) Å
β = 92.19 (3)°
V = 1510.9 (5) Å^3
Z = 4
D_x = 1.320 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 293 (2) K
Block, colourless
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.917, T_{max} = 0.957
3188 measured reflections
2959 independent reflections
1914 reflections with $I > 2\sigma(I)$
R_{int} = 0.094
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.208
S = 1.09
2959 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.09P)^2 + 1.3P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.86	1.97	2.659 (5)	136
N1—H1A···S1^{i}	0.86	2.65	3.511 (3)	174
N2—H2A···O1^{ii}	0.86	2.40	3.093 (5)	138

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

All H atoms were positioned geometrically (C—H = 0.93–0.96 Å and N—H = 0.86 Å) and refined as riding, with U_{iso}(H) = 1.5U_{eq}(C) for the methyl H atoms and 1.2U_{eq}(C,N) for the remaining H atoms.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

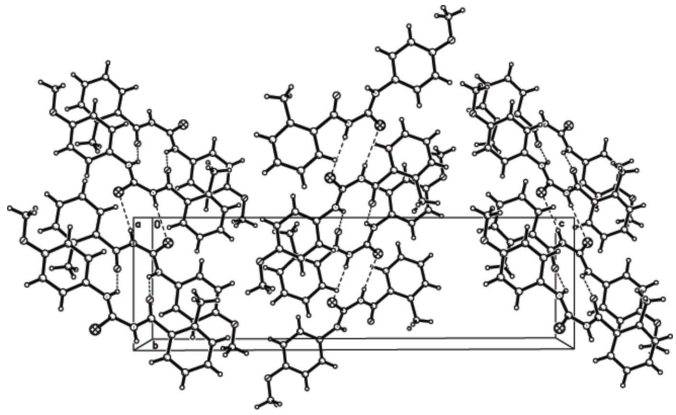


Figure 2
A packing diagram of (I), viewed approximately down the *a* axis. The dashed lines indicate the intermolecular hydrogen bonds.

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References

Allen, F. H., Kennard, O., Watosn, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Cao, Y., Zhao, B., Zhang, Y.-Q. & Zhang, D.-C. (1996). *Acta Cryst.* C**52**, 1772–1774.
Du, Z. X. & Ye, W. F. (2002). *J. Yanbei Normal Univ. (Nat. Sci.)*, **18**, 7–11.
Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Feng, X. M., Chen, R., Yang, W. D. & Zhang, Z. Y. (1992). *Chem. J. Chin. Univ.* **13**, 187–190.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Koch, K. R. (2001). *Coord. Chem. Rev.* **216–217**, 473–488.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sun, C. W., Huang, H., Feng, M. Q., Shi, X. L., Zhang, X. D. & Zhou, P. (2006). *Bioorg. Med. Chem. Lett.* **16**, 162–166.
Xu, X. Y., Qian, X. H., Li, Z., Huang, Q. C. & Chen, G. (2003). *J. Fluorine Chem.* **121**, 51–54.
Yamin, B. M. & Yusof, M. S. M. (2003). *Acta Cryst.* E**59**, o151–o152.