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N-(2,4-Dichlorophenoxyacetyl)-*N*′-(4-nitrophenyl)thiourea

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.064
wR factor = 0.170
Data-to-parameter ratio = 14.7

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

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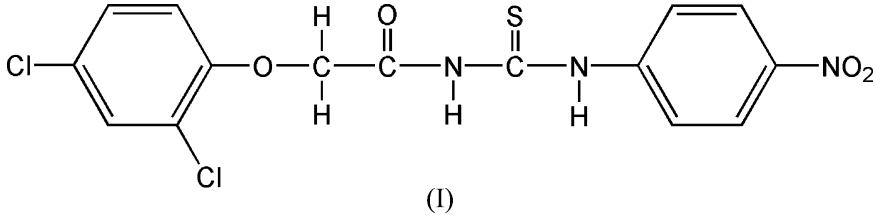
In the crystal structure of the title compound, $C_{15}H_{11}Cl_2N_3O_4S$, there are two intramolecular N—H···O and one C—H···S hydrogen bonds and a weak intermolecular C—H···O hydrogen bond.

Comment

The title compound, (I), belongs to the class of aroylthiourea compounds, which have extensive biological properties, such as antiviral, herbicidal, pesticidal and plant-growth-regulating activity (Xu *et al.*, 2003; Sun *et al.*, 2006; Du *et al.*, 2002). Its structure is described here as part of our work studying the relationship between structure and biological activity.



(I)

A view of the molecular structure of (I) is given in Fig. 1, and selected geometric parameters are listed in Table 1. The C9—S, C9—N1 and C9—N2 bond lengths are 1.644 (5), 1.395 (5) and 1.350 (5) Å, respectively, comparable with those in *N*-(4-methylbenzoyl)-*N*′-(4-nitrophenyl)thiourea [1.649 (2), 1.372 (3) and 1.339 (3) Å, respectively; Yusof *et al.*, 2006].

The crystal structure of (I) contains two intramolecular N—H···O and one C—H···S hydrogen bonds, and a weak intermolecular C—H···O hydrogen bond. The intramolecular interactions form a five-membered N1/C8/C7/O1/H1*A* ring and two six-membered rings, C8/N1/C9/C15/H15*A* and O2/C8/N1/C9/N2/H2*A*.

Experimental

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

Crystal data

$C_{15}H_{11}Cl_2N_3O_4S$
M_r = 400.23
Monoclinic, *C*2/*c*
a = 23.315 (5) Å
b = 8.3190 (17) Å
c = 18.452 (4) Å
β = 109.18 (3)°
V = 3380.2 (14) Å^3
Z = 8
D_x = 1.573 Mg m^{-3}
Mo *K*α radiation
μ = 0.53 mm^{-1}
T = 293 (2) K
Prism, yellow
0.40 × 0.20 × 0.20 mm

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Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (*XCAD4*; Harms & Wocadlo, 1995)
T_{min} = 0.815, T_{max} = 0.901
3400 measured reflections
3316 independent reflections
1943 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.170
S = 1.08
3316 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 3.2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S—C9	1.644 (5)	N2—C9	1.350 (5)
O1—C4	1.349 (5)	N2—C10	1.412 (5)
O1—C7	1.413 (5)	C7—C8	1.509 (6)
N1—C8	1.355 (5)	C10—C15	1.371 (6)
N1—C9	1.395 (5)	C10—C11	1.381 (5)
C4—O1—C7	119.5 (3)	N1—C8—C7	115.8 (4)
C8—N1—C9	130.2 (4)	N2—C9—N1	113.0 (4)
C9—N2—C10	131.2 (4)	N2—C9—S	129.5 (3)
O1—C7—C8	108.8 (4)	N1—C9—S	117.5 (3)
O2—C8—N1	125.4 (4)	C15—C10—N2	125.6 (4)
O2—C8—C7	118.7 (4)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.86	2.09	2.559 (5)	114
N2—H2A···O2	0.86	1.95	2.678 (5)	142
C11—H11A···O2^{i}	0.93	2.45	3.305 (5)	152
C15—H15A···S	0.93	2.56	3.225 (5)	129

Symmetry code: (i) $-x+1, y, -z-\frac{1}{2}$.

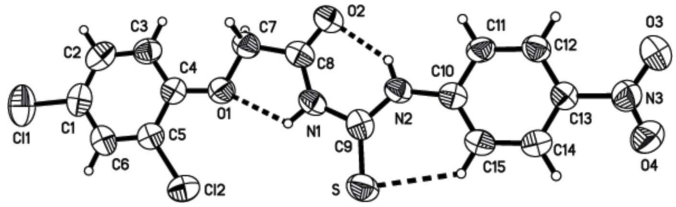

Figure 1
View of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate hydrogen bonds.

All H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93 or 0.97 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C,N).

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*.

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References

Bruker (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
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.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
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.
Yusof, M. S. M., Hamid, M. A., Ramli, R. N. H. R. & Yamin, B. M. (2006). *Acta Cryst.* E**62**, o2131–o2132.
Zhang, Z. Y. & Lin, H. X. (1992). *Chem. J. Chin. Univ.* **13**, 936–937.