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Ethoxycarbonylmethyl 3-(2-chlorobenzylidene)-dithiocarbazate

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The title compound, $C_{12}H_{13}ClN_2O_2S_2$, is a new Schiff base derived from ring opening of *N*-aminorhodanine. It is prepared by reaction of *N*-aminorhodanine and 2-chlorobenzaldehyde in an ethanol solution in the presence of HCl. In the solid state, intermolecular N—H···O hydrogen bonds link the molecules into chains.

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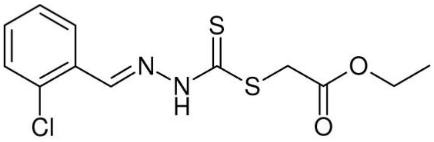
Key indicators

Single-crystal X-ray study
T = 150 K
Mean *σ*(C–C) = 0.002 Å
R factor = 0.029
wR factor = 0.067
Data-to-parameter ratio = 17.1

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

Comment

During the last few decades, there has been considerable interest in the chemistry of Schiff base compounds (Dubey & Vaid, 1991). Schiff bases have been extensively studied for various reasons, one of which is their biological activity (Todeschini *et al.*, 1998; Demirbas, 2004; Rando *et al.*, 2002). Schiff bases containing different donor atoms also find use in analytical applications (Galic *et al.*, 2001; Wyrzykiewicz & Prukah, 1998; Reddy & Lirgappa, 1994). Recently, we have reported the syntheses of some Schiff bases derived from 4-amino-6-methyl-1,2,4-triazine-3-thione-5(2*H*)-one (AMTTO; Tabatabaee *et al.*, 2006) and 4-amino-5-methyl-1,2,4-triazole-3(4*H*)-thione (AMTT), and their use as ligands in Ag^I and Cu^I complexes (Ghassemzadeh *et al.* 2004, 2005, 2006). We report here a new Schiff base, (I), derived from ring opening of *N*-aminorhodanine, prepared by its reaction with 2-chlorobenzaldehyde in ethanol solution in the presence of HCl.



(I)

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles are unexceptional. In the solid state, intermolecular N—H···O hydrogen bonds (Table 1) link the molecules into chains.

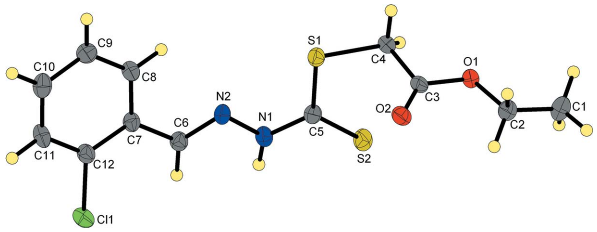


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radius.

Experimental

A solution of *N*-aminorhodanine (4 mmol) in EtOH (20 ml) was treated with 2-chlorobenzaldehyde (6 mmol) and the resulting mixture was acidified with 37% hydrochloric acid (0.2 ml). The reaction mixture was refluxed for 5 h. The solid residue was filtered, washed with cold ethanol (10 ml) and recrystallized from EtOH (yield 89%).

Crystal data

$C_{12}H_{13}ClN_2O_2S_2$
$M_r = 316.81$
Monoclinic, $P2_1/c$
$a = 10.5613$ (18) Å
$b = 16.856$ (3) Å
$c = 8.1013$ (14) Å
$\beta = 96.409$ (14)°
$V = 1433.2$ (4) Å^3
$Z = 4$
$D_x = 1.468$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.56$ mm^{-1}
$T = 150$ (2) K
Prism, yellow
0.20 × 0.15 × 0.10 mm

Data collection

Stoe IPDS-II diffractometer
φ scans
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 2005) $T_{\min} = 0.905$, $T_{\max} = 0.946$
10851 measured reflections
3029 independent reflections
2808 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.028$
$\theta_{\max} = 26.8°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.067$
$S = 1.14$
3029 reflections
177 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0242P)^2 + 0.6651P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.27$ e Å^{-3}
$\Delta\rho_{\min} = -0.17$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$O2$^{\rm i}$	0.85 (2)	2.17 (2)	2.9870 (18)	162.0 (19)

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

H atoms were positioned geometrically, with C—H = 0.95 Å for aromatic, C—H = 0.99 Å for methylene and C—H = 0.98 Å for methyl H atoms, and were allowed to ride during subsequent refinement, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or $1.5U_{\rm eq}$(methyl C). The methyl group was allowed to rotate about its local threefold axis. The H atom of the NH group was located in a difference Fourier map and refined freely with an isotropic displacement parameter.

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-RED32* (Stoe & Cie, 2005); data reduction: *X-RED32*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: X-STEP32 (Stoe & Cie, 2000); software used to prepare material for publication: *SHELXL97*.

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References

Demirbas, A. (2004). *Turk. J. Chem.* **28**, 311–325.
Dubey, S. N. & Vaid, B. K. (1991). *Synth. React. Inorg. Met.-Org. Chem.* **21**(9), 1299–1311.
Galic, N., Galic, N., Peric, B., Kojic-Prodic, B. & Cimerman, Z. (2001). *J. Med. Chem.* **559**, 187–94.
Ghassemzadeh, M., Sharifi, A., Malakootikhah, J., Neumüller, B. & Iravani, E. (2004). *Inorg. Chim. Acta*, **357**, 2245–2252.
Ghassemzadeh, M., Tabatabaee, M., Pooramini, M. M., Heravi, M. M., Eslami, A. & Neumüller, B. (2006). *Z. Anorg. Allg. Chem.* **632**, 786–792.
Ghassemzadeh, M., Tabatabaee, M., Solimani, S. & Neumüller, B. (2005). *Z. Anorg. Allg. Chem.* **631**, 1871–1876.
Rando, D. G., Sato, D. N., Siqueira, L., Malvezzi, A., Leite, C. Q. F., Amaral, A. T., Ferreira, F. I. & Tavares, L. C. (2002). *Bioorg. Med. Chem.* **10**, 557–560.
Reddy, H. & Lirgappa, Y. (1994). *Indian J. Heterocycl. Chem.* **33**, 919–923.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Stoe & Cie (2000). *X-STEP32*. Version 1.07e. Stoe & Cie, Darmstadt, Germany.
Stoe & Cie (2005). *X-AREA* (Version 1.31), *X-RED*32 (Version 1.28b) and *X-SHAPE* (Version 2.05). Stoe & Cie, Darmstadt, Germany.
Tabatabaee, M., Ghassemzadeh, M., Zarabi, B. & Neumüller, B. (2006). *Z. Naturforsch. Teil B*, **61**, 1421–1425.
Todeschini, A. R., Miranda, A. N., Silva, K. C. M., Parrini, S. C. & Barreiro, E. (1998). *Eur. J. Med. Chem.* **33**, 189–199.
Wyrzykiewicz, E. & Prukah, D. (1998). *J. Heterocycl. Chem.* **35**, 381–87.

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