

3-[6-(2,4-Dichlorophenyl)-7H-1,2,4-triazolo-  
[3,4-*b*][1,3,4]thiadiazin-3-yl]propan-1-olKai-Huang Zou,<sup>a,b</sup> Li-Xue  
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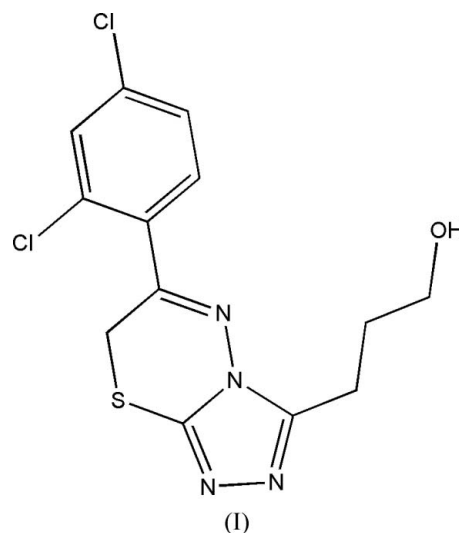
## Key indicators

Single-crystal X-ray study  
*T* = 298 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
*R* factor = 0.048  
*wR* factor = 0.142  
Data-to-parameter ratio = 13.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title compound,  $\text{C}_{13}\text{H}_{12}\text{Cl}_2\text{N}_4\text{OS}$ , the triazole and benzene rings are planar, while the six-membered thiadiazine ring has a screw-boat conformation. Intermolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds form chains which enhance the stability of the crystal structure.

## Comment

1,2,4-Triazole and its derivatives have attracted considerable attention over the past two decades due to their biological activities (Turan *et al.*, 1999; Nadkarni *et al.*, 2001). 1,2,4-Triazole derivatives are used as ingredients in several anti-allergic, antiviral, antibacterial and other drugs (Hui *et al.*, 2001; Chiara *et al.*, 1998). A literature survey reveals that there are not many examples of triazoles fused with thiadiazines. A large number of triazolothiadiazines have been shown to exhibit antimicrobial (Feng *et al.*, 1992) and diuretic (Mohan & Anjaneyulu, 1987) properties and to act as photographic couplers (Holla *et al.*, 2001). In our continued search for new triazole compounds with higher bioactivity, the title compound, (I), was synthesized and characterized by X-ray single-crystal diffraction.



In the title compound, atoms C9 and S1 deviate by 0.615 (4) and 1.186 (4) Å, respectively, from the mean plane through atoms C7, C8, N1 and N2. The triazole and benzene rings are planar, while the six-membered thiadiazine ring has a screw-boat conformation (Fig. 1). The triazole bond lengths exhibit normal values (Jin *et al.*, 2004). Intermolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds link the molecules into chains (Fig. 2 and Table 1).

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## Experimental

The starting materials for the thiocarbohydrazide were carbon disulfide and hydrazine hydrate. 4-Amino-3-(3-hydroxypropyl)-5-mercapto-1,2,4-triazole was prepared by the reaction of 1,4-butyrolactone and thiocarbohydrazide in a pyridine solution, following the method of Xiong *et al.* (2002). A mixture of 4-amino-3-(3-hydroxypropyl)-5-mercapto-1,2,4-triazole (1 mmol) and 2-bromo-1-(2,4-dichlorophenyl)ethanone (1 mmol) in absolute ethanol (20 ml) was refluxed for 7 h. The solid obtained on cooling was filtered off, washed with cold water, dried and recrystallized from ethanol to give compound (I). The purified product was dissolved in 95% ethanol and kept at room temperature for 5 d, whereupon single crystals of (I) were formed.

## Crystal data

$C_{13}H_{12}Cl_2N_4OS$	$V = 733.82(11) \text{ \AA}^3$
$M_r = 343.23$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.553 \text{ Mg m}^{-3}$
$a = 8.1605(7) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.5239(8) \text{ \AA}$	$\mu = 0.59 \text{ mm}^{-1}$
$c = 11.2810(9) \text{ \AA}$	$T = 298(2) \text{ K}$
$\alpha = 95.237(2)^\circ$	Block, colorless
$\beta = 105.340(2)^\circ$	$0.38 \times 0.26 \times 0.20 \text{ mm}$
$\gamma = 101.205(2)^\circ$	

## Data collection

Bruker APEX area-detector diffractometer	3875 measured reflections
$\varphi$ and $\omega$ scan	2564 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2002)	2317 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.808$ , $T_{\max} = 0.892$	$R_{\text{int}} = 0.011$
	$\theta_{\text{max}} = 25.0^\circ$

## Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0816P)^2 + 0.4287P]$
$R[F^2 > 2\sigma(F^2)] = 0.048$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.142$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 1.13 \text{ e \AA}^{-3}$
2564 reflections	$\Delta\rho_{\text{min}} = -0.37 \text{ e \AA}^{-3}$
191 parameters	
H-atom parameters constrained	

Table 1

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1\cdots N3^i$	0.82	2.03	2.854 (4)	178

Symmetry code: (i)  $x, y - 1, z$ .

H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of  $Csp^2-H = 0.93 \text{ \AA}$  and  $N-H = 0.92 \text{ \AA}$  with  $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{parent atom})$ , and  $Csp^3-H = 0.96$  or  $0.97 \text{ \AA}$  with  $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{parent atom})$ . The deepest hole is  $0.57 \text{ \AA}$  from atom O1 and the highest peak is  $0.44 \text{ \AA}$  from atom H13A.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2002); software used to prepare material for publication: SHELXL97.

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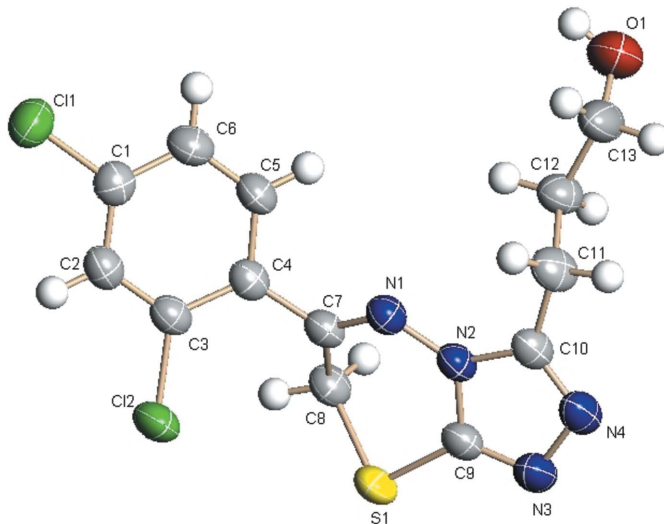


Figure 1

The molecular structure of (I) with the atom numbering, showing displacement ellipsoids drawn at the 30% probability level.

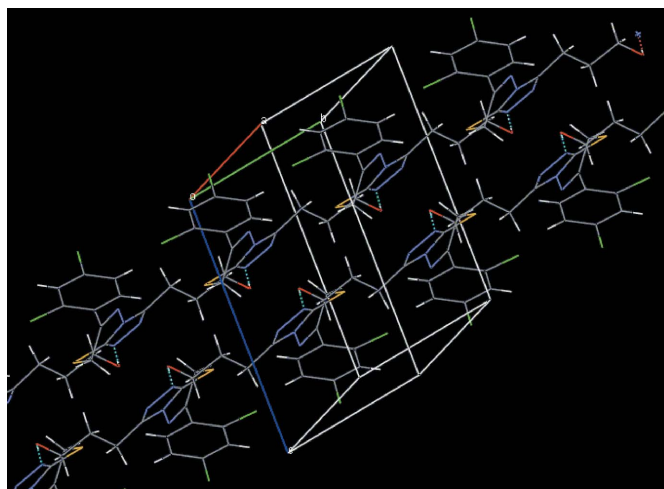


Figure 2

Chains formed by hydrogen-bonding interactions (dashed lines).

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