2-{5-[(1*H*-1,2,4-Triazol-1-yl)methyl]-1,3,4-oxadiazol-2-ylthio}-1-(2,4-dichlorophenyl)-ethanone

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In the molecule of the title compound, $C_{13}H_9Cl_2N_5O_2S$, prepared by the reaction of 5-[(1*H*-1,2,4-triazol-1-yl)methyl]-1,3,4-oxadiazole-2-thiol and 2-bromo-1-(2,4-dichlorophen-yl)ethanone, the 1,3,4-oxadiazole ring makes dihedral angles of 50.56 (2) and 82.95 (4)°, respectively, with the benzene and triazole rings. Weak intermolecular C—H···N hydrogen bonds link the molecules into zigzag chains extending along the *b* axis.

Comment

Triazole and 1,3,4-oxadiazole derivatives are known to possess a wide spectrum of insecticidal and fungicidal activities (Pachhamia & Parikh, 1988; Xu *et al.*, 2002). In our search for compounds with better properties, the title compound, (I) (Fig. 1), has been synthesized. We report here its crystal structure.

(I)
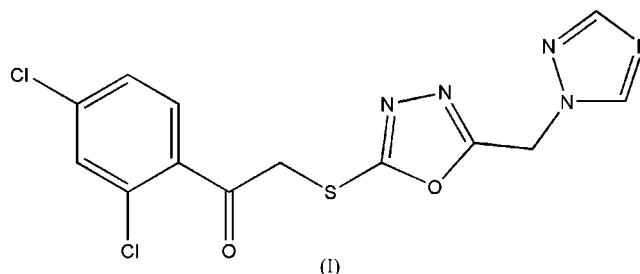
In (I), the bond lengths and angles of the triazole and 1,3,4-oxadiazole rings (Table 1) are in a good agreement with the values quoted in previous reports (Xu *et al.*, 2005; Zhang *et al.*, 2002). Atoms C11 and S1 lie in the plane of the 1,3,4-oxadiazole ring (C9/C10/N1/N2/O1). The dihedral angles formed by the benzene (C3–C8/Cl1/Cl2) and triazole (C12/C13/N3–N5) rings with the 1,3,4-oxadiazole ring are 50.56 (2) and 82.95 (4)°, respectively. Weak intermolecular C—H···N hydrogen bonds (Table 2) link the molecules into zigzag chains extending along the *b* axis. The relatively short distance $Cg1\cdots Cg2^{ii}$ of 3.702 (2) Å, where $Cg1$ and $Cg2$ denote the centroids of the triazole and benzene rings, respectively [symmetry code: (ii) $1 + x, \frac{1}{2} - y, -\frac{1}{2} + z$], indicates a possible π–π stacking interaction. The crystal packing (Fig. 2) is mainly stabilized by van der Waals forces.

Experimental

A mixture of 5-[(1*H*-1,2,4-triazol-1-yl)methyl]-1,3,4-oxadiazole-2-thiol (0.02 mol) and 2-bromo-1-(2,4-dichlorophenyl)ethanone (0.02 mol) was stirred in refluxing acetone (15 ml) for 5 h at 327 K to afford the title compound (5.90 g, yield 80%). Single crystals suitable

for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Crystal data

$C_{13}H_9Cl_2N_5O_2S$	$D_x = 1.594$ Mg m^{-3}
$M_r = 370.21$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2652
$a = 7.3130$ (13) Å	reflections
$b = 25.231$ (4) Å	$\theta = 2.6–25.6°$
$c = 8.4269$ (15) Å	$\mu = 0.57$ mm^{-1}
$\beta = 97.217$ (3)°	$T = 294$ (2) K
$V = 1542.5$ (5) Å^3	Block, colorless
$Z = 4$	$0.22 \times 0.16 \times 0.14$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	3149 independent reflections
	2155 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.028$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{max} = 26.4°$
	$h = -7 \rightarrow 9$
$T_{min} = 0.880$, $T_{max} = 0.923$	$k = -28 \rightarrow 31$
8564 measured reflections	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0334P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.040$	$+ 0.996P]$
$wR(F^2) = 0.097$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
3149 reflections	$\Delta\rho_{max} = 0.46$ e Å^{-3}
208 parameters	$\Delta\rho_{min} = -0.35$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

S1—C9	1.730 (3)	N1—C9	1.284 (3)
S1—C1	1.797 (2)	N1—N2	1.417 (3)
O1—C9	1.364 (3)	N2—C10	1.275 (3)
O1—C10	1.366 (3)		
C9—S1—C1	98.68 (12)	C9—O1—C10	101.82 (18)

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···N5^i	0.93	2.41	3.319 (4)	167
C1—H1B···Cl1	0.97	2.48	3.051 (2)	117

Symmetry code: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$.

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); 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, 1999); software used to prepare material for publication: SHELXTL.
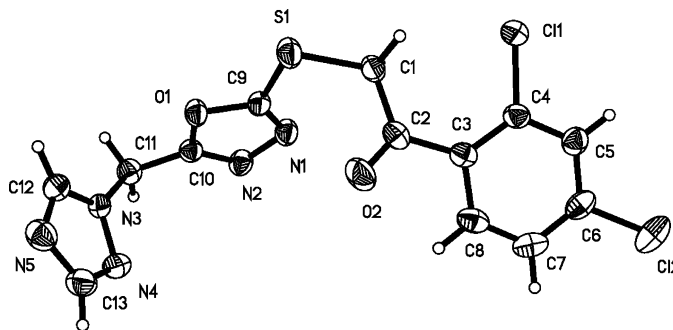

Figure 1
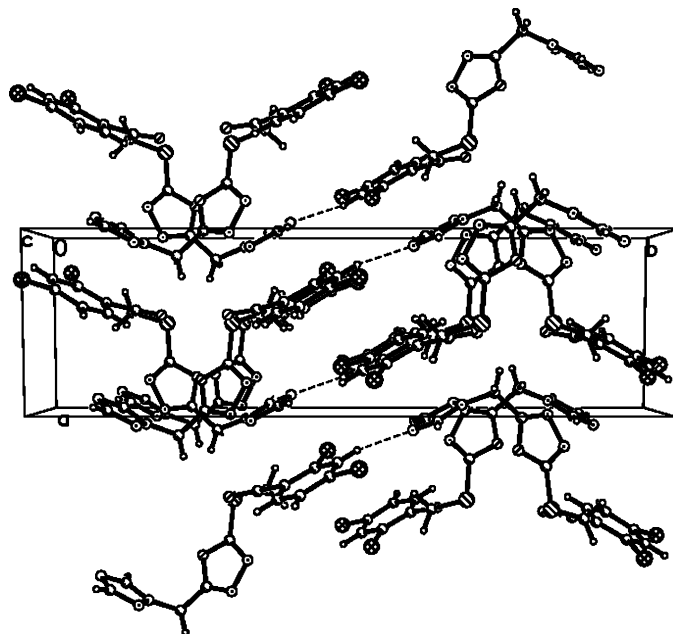View of the title compound (I), with displacement ellipsoids drawn at the 40% probability level.

Figure 2
A packing diagram of the title compound, viewed down the c axis. Hydrogen bonds are shown as dashed lines.

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