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(*Z*)-1-(2,5-Dichlorophenyl)-2-(3-phenylthiazolidin-2-ylidene)ethanone

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.040
wR factor = 0.091
Data-to-parameter ratio = 16.3

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

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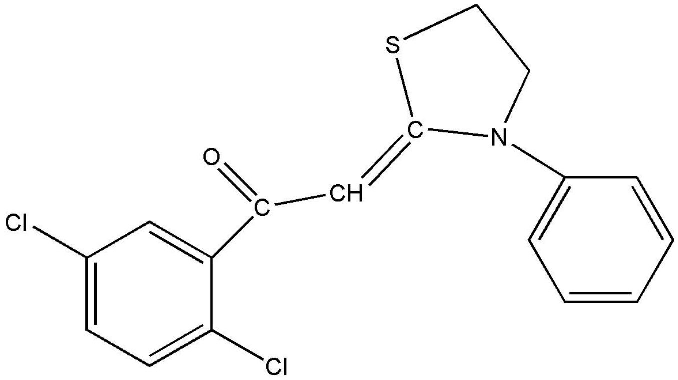
In the title compound, $C_{17}H_{13}Cl_2NOS$, the heterocyclic five-membered ring is essentially planar. The molecules in the crystal structure are stabilized by intermolecular C—H···π interactions and weak intramolecular C—H···Cl hydrogen-bond interactions.

Comment

It has been reported that thiazolidines have insecticidal, fungicidal, herbicidal and acaricidal activities (Austin *et al.*, 2000; Shibata *et al.*, 1999; Walter, 1997). As part of our search for new thiazolidine compounds with better herbicidal and fungicidal activities, the title compound, (I), was synthesized. We report here the crystal structure of (I).



(I)

Bond lengths and angles of the thiazolidine ring (Table 1) are in agreement with the values quoted in a previous report (Xu *et al.*, 2005). The heterocyclic five-membered ring (C1/C2/N1/C3/S1) is essentially planar, with a maximum displacement from the mean plane of 0.016 (4) Å for atom C1. The dihedral angles formed by the Cl1/Cl2/C6–C11 and C12–C17 mean planes with the hetero-ring plane are 39.47 (8) and 61.29 (11)°, respectively.

The molecules in the crystal structure are stabilized by intermolecular C—H···π and weak intramolecular C—H···Cl hydrogen-bond interactions (Table 2).

Experimental

The title compound was prepared by the reaction of 1-(2,5-dichlorophenyl)ethanone (0.01 mol), 1,2-dibromoethane (0.01 mol) and isothiocyanatobenzene (0.01 mol) at 313–318 K for 4 h. Single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

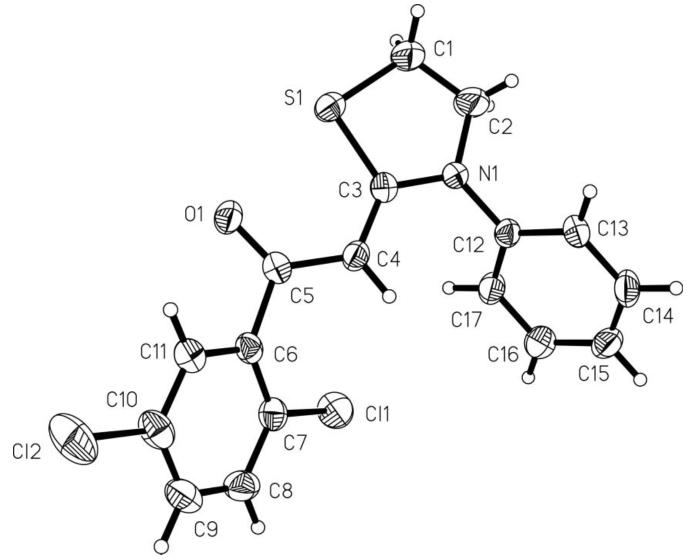


Figure 1
View of the title compound (I), with displacement ellipsoids drawn at the 40% probability level.

Crystal data

$C_{17}H_{13}Cl_2NOS$
$M_r = 350.24$
Orthorhombic, $Fdd2$
$a = 26.088$ (4) Å
$b = 37.204$ (6) Å
$c = 6.5952$ (11) Å
$V = 6401.1$ (19) Å^3
$Z = 16$
$D_x = 1.454$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 2162 reflections
$\theta = 3.2$–23.1°
$\mu = 0.54$ mm^{-1}
$T = 294$ (2) K
Block, yellow
0.42 × 0.28 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.790$, $T_{\max} = 0.879$
8964 measured reflections

3235 independent reflections
2178 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.048$
$\theta_{\max} = 26.4°$
$h = -32 \rightarrow 32$
$k = -46 \rightarrow 23$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.092$
$S = 1.02$
3235 reflections
199 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 1.9653P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}
Absolute structure: Flack (1983), 1443 Friedel pairs
Flack parameter: 0.01 (8)

Table 1
Selected geometric parameters (Å, °).

S1—C3	1.736 (3)	N1—C2	1.430 (4)
S1—C1	1.806 (3)	C1—C2	1.441 (5)
N1—C3	1.356 (4)	C3—C4	1.373 (4)
C3—S1—C1	91.78 (17)	N1—C3—S1	112.1 (2)
C3—N1—C2	115.9 (3)		
C3—S1—C1—C2	−1.7 (4)	S1—C1—C2—N1	1.7 (5)

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

Cg1, Cg2 and Cg3 are the centroids of the S1/N1/C1–C3, C6–C11 and C12–C17 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···Cl1	0.93	2.74	3.169 (5)	109
C16—H16···$Cg1^{\rm i}$	0.93	3.19	3.800 (4)	125
C13—H13···$Cg2^{\rm ii}$	0.93	3.10	3.727 (1)	127
C9—H9···$Cg3^{\rm iii}$	0.93	2.91	3.838 (2)	173

Symmetry codes: (i) $x, y, z+1$; (ii) $x+\frac{1}{4}, -y-\frac{1}{4}, z-\frac{1}{4}$; (iii) $x-1, y, z$.

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 $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$.

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*.

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