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Key indicators

Single-crystal X-ray study
 $T = 294\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.045
 wR factor = 0.126
Data-to-parameter ratio = 12.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**(E)-4-(4-Chlorophenyl)-N-(5-methyl-1,3-benzodioxol-5-ylmethylene)-5-(1H-1,2,4-triazol-1-yl)-1,3-thiazol-2-amine**The title compound, $\text{C}_{19}\text{H}_{12}\text{ClN}_5\text{O}_2\text{S}$, has been synthesized as a potential fungicidal agent. The dihedral angle between the thiazole and triazole rings is $38.5(1)^\circ$.Received 7 December 2005
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Comment

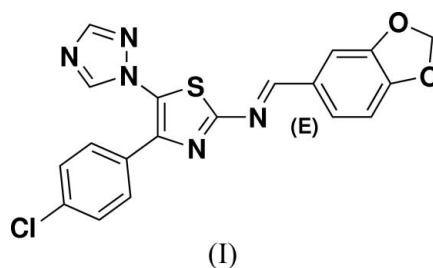
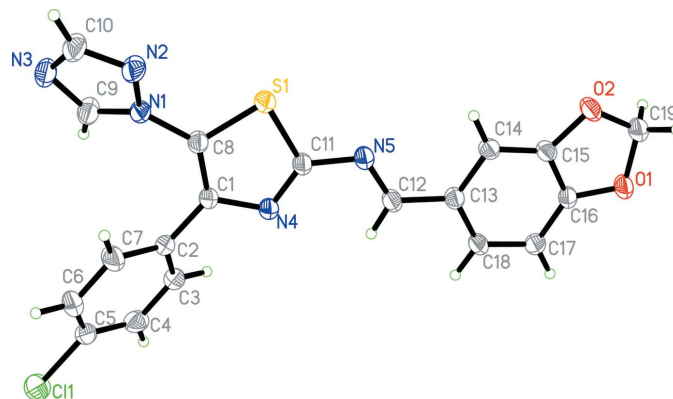
Thiazole derivatives are reported to exhibit diverse biological activities, such as antitubercular, bacteriostatic and fungistatic activities (Smia *et al.*, 2000). In search of novel thiazole compounds with potent fungicidal activities, we have sought to synthesize such 2-aminothiazole compounds containing 1H-1,2,4-triazole units. We report here the crystal structure of the title compound, (I).The methylbenzo[1,2-*d*]-1,3-dioxolyl and thiazole rings are nearly coplanar, with a dihedral angle between them of $3.0(1)^\circ$, whereas the triazole and 4-chlorophenyl rings are twisted with respect to the thiazole ring by $38.5(1)$ and $36.0(1)^\circ$, respectively.The occurrence of weak $\text{C}-\text{H}\cdots\text{O}$ interactions (Table 1) results in the formation of pseudo-dimers arranged around inversion centres.

Figure 1

A molecular view of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Experimental

2-Amino-4-(4-chlorophenyl)-5-(1*H*-1,2,4-triazol-1-yl)-1,3-thiazole (0.42 g, 1.5 mmol) and heliotropin (0.22 g, 1.5 mmol) were mixed in benzene (20 ml). Three drops of piperidine were added to the mixed solution. The solution was then heated and refluxed in a 50 ml flask equipped with a Dean–Stark trap condenser until no water appeared (5 h). Concentration of the reaction solution and chromatography on a silica-gel column using ethyl acetate–petroleum ether (1:3) as eluent gave the title compound (0.51 g, yield 83.2%). Single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{19}H_{12}ClN_5O_2S$	$Z = 2$
$M_r = 409.85$	$D_x = 1.512 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.8260 (19) \text{ \AA}$	Cell parameters from 1873 reflections
$b = 8.929 (2) \text{ \AA}$	$\theta = 2.9\text{--}26.3^\circ$
$c = 14.221 (3) \text{ \AA}$	$\mu = 0.36 \text{ mm}^{-1}$
$\alpha = 94.871 (4)^\circ$	$T = 294 (2) \text{ K}$
$\beta = 92.332 (4)^\circ$	Block, yellow
$\gamma = 114.170 (4)^\circ$	$0.26 \times 0.20 \times 0.16 \text{ mm}$
$V = 900.2 (4) \text{ \AA}^3$	

Data collection

Bruker SMART CCD area-detector diffractometer	3160 independent reflections
φ and ω scans	2302 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.029$
$T_{\text{min}} = 0.910$, $T_{\text{max}} = 0.945$	$\theta_{\text{max}} = 25.0^\circ$
4582 measured reflections	$h = -9 \rightarrow 9$
	$k = -10 \rightarrow 9$
	$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0622P)^2 + 0.3304P]$
$R[F^2 > 2\sigma(F^2)] = 0.045$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.127$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.32 \text{ e \AA}^{-3}$
3160 reflections	$\Delta\rho_{\text{min}} = -0.41 \text{ e \AA}^{-3}$
253 parameters	
H-atom parameters constrained	

Table 1

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

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
$C9\text{--}H9\cdots O1^i$	0.93	2.52	3.371 (4)	152

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

All H atoms were placed in calculated positions and treated as riding on their parent C atoms, with $C\text{--}H = 0.93 \text{ \AA}$ (C_{aromatic}) and $C\text{--}H = 0.97 \text{ \AA}$ ($C_{\text{methylene}}$), and with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$.

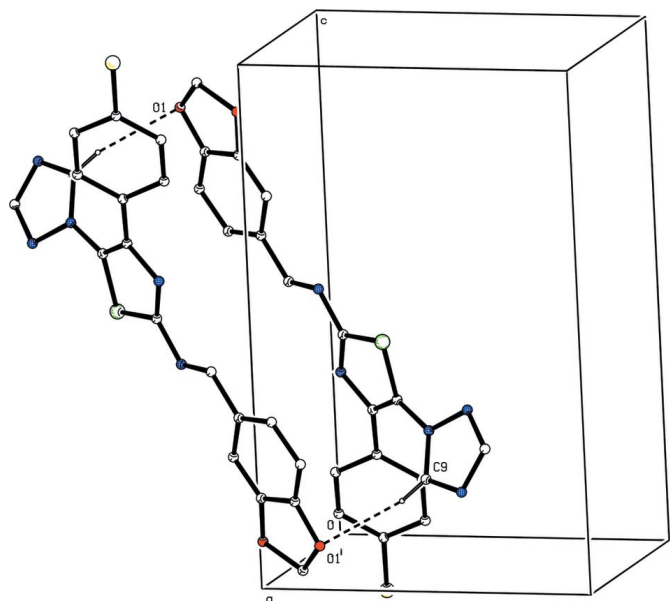


Figure 2

A view showing the formation of pseudo-dimers through weak $C\text{--}H\cdots O$ interactions (dashed lines). H atoms not involved in hydrogen bonds have been omitted for clarity.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1999); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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