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1-(4-Chlorophenyl)-3-{5-[(*E*)-2-phenylethenyl]-1,3,4-thiadiazol-2-yl}urea

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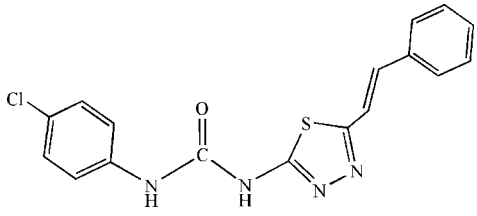
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.068; wR factor = 0.154; data-to-parameter ratio = 16.6.

In the title compound, $C_{17}H_{13}ClN_4OS$, the 1,3,4-thiadiazole ring makes dihedral angles of 9.70 (15) and 7.22 (10)° with the benzene and phenyl rings, respectively; the dihedral angle between these two rings is 6.37 (19)°. In the crystal, pairs of N—H···N and C—H···O hydrogen bonds between inversion-related molecules result in supramolecular ribbons displaying alternate $R_2^2(8)$ and $R_2^2(14)$ graph-set ring motifs.

Related literature

For the biological activity of urea derivatives, see: Abad *et al.* (2004); Chen *et al.* (2005); Yonova & Stoilkova (2005). For the biological activity of 1,3,4-thiadiazole derivatives, see: Guzeldemirci & Kucukbasmaci (2010); Song & Tan (2008); Zou *et al.* (2002). For the synthesis, see: Song *et al.* (2007).



Experimental

Crystal data

$C_{17}H_{13}ClN_4OS$
M_r = 356.82
Monoclinic, $P2_1/c$
a = 11.2399 (6) Å
b = 4.1032 (2) Å
c = 35.2497 (16) Å
β = 91.525 (4)°
V = 1625.12 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 298 K
0.40 × 0.06 × 0.02 mm

Data collection

Bruker SMART CCD area-detector diffractometer
10860 measured reflections
3708 independent reflections
2081 reflections with $I > 2\sigma(I)$
R_{int} = 0.091

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.154
S = 1.01
3708 reflections
223 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.93	2.55	3.432 (4)	159
N2—H2A···N3^{ii}	0.82 (4)	2.03 (4)	2.848 (4)	174 (3)

Symmetry codes: (i) $-x+2, -y, -z$; (ii) $-x+1, -y+2, -z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2664).

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supplementary materials

Acta Cryst. (2011). E**67**, o510 [**doi:10.1107/S1600536811002479**]

1-(4-Chlorophenyl)-3-{5-[(*E*)-2-phenylethenyl]-1,3,4-thiadiazol-2-yl}urea

X.-H. Zhan and Z.-Y. Wang

Comment

Urea derivatives have attracted much attention on the account of their interesting biological effects, such as insecticidal, fungicidal, herbicidal and plant-growth regulating activities (Abad *et al.*, 2004; Chen *et al.*, 2005), especially cytokinin acyivity (Yonova & Stoilkova, 2005). 1,3,4-Thiadiazole derivatives are known to exhibit a wide range of biological activities (Zou *et al.*, 2002; Song & Tan, 2008; Guzeldemirci & Kucukbasmaci, 2010). In view of our extensive interest and as a continuing search for new urea-type cytokinins, we investigate the urea derivatives incorporating a 1,3,4-thiadiazole nucleus, including the title compound.

The crystal structure (Fig.1) revealed that the title molecule which consists of three rings is approximately planar, the dihedral angles formed by the thiadiazole ring with the chlorophenyl and vinylphenyl rings being only 9.70 (15) and 7.22 (10)°, respectively, and the styryl moiety assumes a *trans*-configuration about C10═C11 double bond of the vinyl moiety. All bond lengths and angles are as expected. In the crystal structure, intermolecular N—H···N and C—H···O hydrogen bonds occurring between centrosymmetrically related molecules result in the formation of ribbons displaying alternate rings of graph-set motifs $R_2^2(8)$ and $R_2^2(14)$, as shown in Fig. 2 and Table 1.

Experimental

The title compound was prepared according to the procedure of Song *et al.* (2007). Suitable crystals were obtained by vapor diffusion of methanol in DMF at room temperature (m.p. >573 K). Elemental analysis: analysis calculated for $C_{17}H_{13}ClN_4OS$: C 57.22, H 3.67, N 15.70%; found: C 57.45, H 3.56, N 15.82%.

Refinement

C-bound H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H = 0.93 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$. N-bound H atoms were freely refined [refined distances 0.82 (4) and 0.86 (3) Å].

Figures

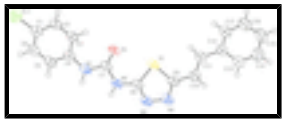

Fig. 1. View of the title molecule, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

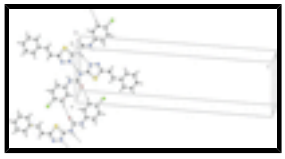

Fig. 2. A partial packing diagram of the title molecule. Hydrogen bonds are indicated by dashed lines.

1-(4-Chlorophenyl)-3-{5-[(*E*)-2-phenylethenyl]-1,3,4-thiadiazol-2-yl}urea

Crystal data

$C_{17}H_{13}ClN_4OS$	$F(000) = 736$
	$D_x = 1.458$ Mg m^{-3}
$M_r = 356.82$	$D_m = 1.459$ Mg m^{-3}
	D_m measured by not measured
Monoclinic, $P2_1/c$	Melting point > 573 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 11.2399$ (6) Å	Cell parameters from 1521 reflections
$b = 4.1032$ (2) Å	$\theta = 2.9$–$23.2°$
$c = 35.2497$ (16) Å	$\mu = 0.38$ mm^{-1}
$\beta = 91.525$ (4)°	$T = 298$ K
$V = 1625.12$ (14) Å^3	Block, colorless
$Z = 4$	0.40 × 0.06 × 0.02 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2081 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.091$
graphite	$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$
φ and ω scans	$h = -14 \rightarrow 14$
10860 measured reflections	$k = -5 \rightarrow 5$
3708 independent reflections	$l = -45 \rightarrow 35$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.068$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.154$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
3708 reflections	$(\Delta/\sigma)_{max} = 0.001$
223 parameters	$\Delta\rho_{max} = 0.31$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.20$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations

between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.9546 (3)	−0.0487 (8)	−0.10673 (10)	0.0517 (9)
C2	0.9869 (3)	0.0032 (9)	−0.06905 (10)	0.0559 (10)
H2	1.0585	−0.0780	−0.0592	0.067*
C3	0.9118 (3)	0.1766 (8)	−0.04629 (10)	0.0519 (9)
H3	0.9330	0.2130	−0.0210	0.062*
C4	0.8049 (3)	0.2972 (8)	−0.06083 (10)	0.0440 (8)
C5	0.7739 (3)	0.2341 (9)	−0.09865 (10)	0.0536 (9)
H5	0.7012	0.3078	−0.1085	0.064*
C6	0.8486 (3)	0.0657 (9)	−0.12150 (10)	0.0565 (10)
H6	0.8277	0.0291	−0.1468	0.068*
C7	0.7271 (3)	0.5485 (8)	−0.00213 (10)	0.0468 (8)
C8	0.6130 (3)	0.8377 (8)	0.04418 (10)	0.0458 (8)
C9	0.5972 (3)	0.9536 (8)	0.10951 (9)	0.0470 (8)
C10	0.6089 (3)	0.9901 (8)	0.15047 (10)	0.0499 (9)
H10	0.5513	1.1121	0.1626	0.060*
C11	0.6956 (3)	0.8619 (8)	0.17178 (10)	0.0491 (9)
H11	0.7501	0.7342	0.1591	0.059*
C12	0.7170 (3)	0.8949 (8)	0.21285 (10)	0.0505 (9)
C13	0.6371 (4)	1.0434 (9)	0.23675 (11)	0.0639 (10)
H13	0.5660	1.1267	0.2268	0.077*
C14	0.6625 (5)	1.0679 (11)	0.27489 (12)	0.0839 (13)
H14	0.6079	1.1654	0.2907	0.101*
C15	0.7677 (5)	0.9501 (11)	0.28999 (12)	0.0881 (15)
H15	0.7843	0.9683	0.3159	0.106*
C16	0.8480 (4)	0.8058 (11)	0.26689 (13)	0.0810 (13)
H16	0.9197	0.7273	0.2770	0.097*
C17	0.8222 (4)	0.7772 (9)	0.22848 (11)	0.0656 (11)
H17	0.8768	0.6767	0.2129	0.079*
Cl1	1.05145 (9)	−0.2566 (3)	−0.13606 (3)	0.0742 (4)
N1	0.7246 (2)	0.4851 (7)	−0.04021 (8)	0.0500 (8)
H1A	0.670 (3)	0.583 (8)	−0.0530 (9)	0.060*
N2	0.6343 (3)	0.7450 (8)	0.00788 (9)	0.0540 (8)
H2A	0.588 (3)	0.822 (8)	−0.0081 (10)	0.065*
N3	0.5194 (2)	1.0175 (7)	0.05141 (8)	0.0548 (8)
N4	0.5103 (2)	1.0847 (7)	0.08984 (8)	0.0539 (8)
O1	0.7993 (2)	0.4425 (6)	0.02092 (6)	0.0620 (7)
S1	0.69949 (7)	0.7370 (2)	0.08328 (2)	0.0497 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.045 (2)	0.051 (2)	0.060 (2)	−0.0060 (17)	−0.0008 (18)	0.0119 (18)
C2	0.0382 (19)	0.064 (2)	0.065 (3)	0.0002 (18)	−0.0084 (18)	0.019 (2)
C3	0.042 (2)	0.065 (2)	0.047 (2)	−0.0022 (17)	−0.0103 (16)	0.0139 (18)
C4	0.0360 (17)	0.046 (2)	0.050 (2)	−0.0055 (15)	−0.0075 (15)	0.0151 (17)
C5	0.043 (2)	0.064 (2)	0.052 (2)	−0.0041 (18)	−0.0138 (17)	0.012 (2)
C6	0.057 (2)	0.065 (2)	0.047 (2)	−0.0064 (19)	−0.0108 (19)	0.0081 (19)
C7	0.0388 (19)	0.051 (2)	0.050 (2)	−0.0031 (16)	−0.0126 (16)	0.0128 (18)
C8	0.0393 (19)	0.050 (2)	0.048 (2)	−0.0026 (15)	−0.0126 (15)	0.0128 (17)
C9	0.0367 (18)	0.052 (2)	0.052 (2)	−0.0047 (15)	−0.0042 (16)	0.0126 (17)
C10	0.0432 (19)	0.054 (2)	0.053 (2)	−0.0010 (17)	0.0034 (17)	0.0024 (18)
C11	0.048 (2)	0.049 (2)	0.051 (2)	−0.0004 (16)	−0.0034 (17)	0.0044 (17)
C12	0.057 (2)	0.050 (2)	0.044 (2)	−0.0060 (17)	−0.0064 (18)	0.0063 (17)
C13	0.071 (3)	0.068 (3)	0.053 (3)	0.007 (2)	−0.001 (2)	0.001 (2)
C14	0.120 (4)	0.074 (3)	0.059 (3)	0.007 (3)	0.012 (3)	−0.009 (2)
C15	0.142 (5)	0.071 (3)	0.051 (3)	−0.006 (3)	−0.023 (3)	−0.001 (2)
C16	0.099 (4)	0.076 (3)	0.066 (3)	0.003 (3)	−0.025 (3)	0.003 (3)
C17	0.070 (3)	0.072 (3)	0.054 (2)	0.007 (2)	−0.011 (2)	0.004 (2)
Cl1	0.0655 (7)	0.0789 (7)	0.0785 (8)	0.0047 (5)	0.0083 (5)	0.0018 (6)
N1	0.0393 (16)	0.060 (2)	0.0493 (19)	0.0041 (14)	−0.0180 (14)	0.0090 (15)
N2	0.0420 (17)	0.070 (2)	0.049 (2)	0.0067 (15)	−0.0162 (13)	0.0101 (17)
N3	0.0385 (16)	0.071 (2)	0.0543 (19)	0.0026 (15)	−0.0145 (14)	0.0089 (16)
N4	0.0385 (16)	0.066 (2)	0.057 (2)	−0.0004 (14)	−0.0077 (14)	0.0098 (16)
O1	0.0511 (15)	0.0825 (18)	0.0513 (15)	0.0170 (13)	−0.0186 (12)	0.0107 (14)
S1	0.0397 (5)	0.0609 (6)	0.0479 (5)	0.0024 (4)	−0.0117 (4)	0.0111 (5)

Geometric parameters (Å, °)

C1—C6	1.370 (4)	C9—S1	1.739 (3)
C1—C2	1.384 (5)	C10—C11	1.324 (4)
C1—Cl1	1.744 (4)	C10—H10	0.9300
C2—C3	1.378 (5)	C11—C12	1.468 (4)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.385 (4)	C12—C17	1.379 (5)
C3—H3	0.9300	C12—C13	1.388 (5)
C4—C5	1.393 (5)	C13—C14	1.370 (5)
C4—N1	1.404 (4)	C13—H13	0.9300
C5—C6	1.366 (5)	C14—C15	1.372 (6)
C5—H5	0.9300	C14—H14	0.9300
C6—H6	0.9300	C15—C16	1.366 (6)
C7—O1	1.214 (4)	C15—H15	0.9300
C7—N1	1.367 (4)	C16—C17	1.382 (5)
C7—N2	1.372 (4)	C16—H16	0.9300
C8—N3	1.316 (4)	C17—H17	0.9300
C8—N2	1.362 (4)	N1—H1A	0.86 (3)
C8—S1	1.716 (3)	N2—H2A	0.82 (4)

C9—N4	1.299 (4)	N3—N4	1.389 (4)
C9—C10	1.454 (4)		
C6—C1—C2	121.0 (3)	C10—C11—C12	128.5 (3)
C6—C1—Cl1	119.5 (3)	C10—C11—H11	115.8
C2—C1—Cl1	119.5 (3)	C12—C11—H11	115.8
C3—C2—C1	119.3 (3)	C17—C12—C13	118.2 (3)
C3—C2—H2	120.4	C17—C12—C11	118.6 (3)
C1—C2—H2	120.4	C13—C12—C11	123.2 (3)
C2—C3—C4	120.5 (3)	C14—C13—C12	120.4 (4)
C2—C3—H3	119.7	C14—C13—H13	119.8
C4—C3—H3	119.7	C12—C13—H13	119.8
C3—C4—C5	118.7 (3)	C13—C14—C15	120.6 (4)
C3—C4—N1	124.6 (3)	C13—C14—H14	119.7
C5—C4—N1	116.8 (3)	C15—C14—H14	119.7
C6—C5—C4	121.1 (3)	C16—C15—C14	119.8 (4)
C6—C5—H5	119.4	C16—C15—H15	120.1
C4—C5—H5	119.4	C14—C15—H15	120.1
C5—C6—C1	119.4 (3)	C15—C16—C17	119.7 (4)
C5—C6—H6	120.3	C15—C16—H16	120.1
C1—C6—H6	120.3	C17—C16—H16	120.1
O1—C7—N1	125.8 (3)	C12—C17—C16	121.1 (4)
O1—C7—N2	122.6 (3)	C12—C17—H17	119.4
N1—C7—N2	111.6 (3)	C16—C17—H17	119.4
N3—C8—N2	120.0 (3)	C7—N1—C4	128.1 (3)
N3—C8—S1	114.7 (3)	C7—N1—H1A	115 (2)
N2—C8—S1	125.3 (3)	C4—N1—H1A	117 (2)
N4—C9—C10	122.3 (3)	C8—N2—C7	124.0 (3)
N4—C9—S1	115.2 (3)	C8—N2—H2A	114 (2)
C10—C9—S1	122.5 (2)	C7—N2—H2A	122 (2)
C11—C10—C9	124.6 (3)	C8—N3—N4	112.3 (3)
C11—C10—H10	117.7	C9—N4—N3	111.4 (3)
C9—C10—H10	117.7	C8—S1—C9	86.31 (17)
C6—C1—C2—C3	−0.9 (5)	C13—C12—C17—C16	−0.1 (6)
Cl1—C1—C2—C3	177.9 (2)	C11—C12—C17—C16	179.0 (3)
C1—C2—C3—C4	0.2 (5)	C15—C16—C17—C12	0.7 (6)
C2—C3—C4—C5	1.2 (5)	O1—C7—N1—C4	−2.2 (6)
C2—C3—C4—N1	−177.8 (3)	N2—C7—N1—C4	179.4 (3)
C3—C4—C5—C6	−2.0 (5)	C3—C4—N1—C7	−9.2 (5)
N1—C4—C5—C6	177.1 (3)	C5—C4—N1—C7	171.7 (3)
C4—C5—C6—C1	1.4 (5)	N3—C8—N2—C7	−177.6 (3)
C2—C1—C6—C5	0.1 (5)	S1—C8—N2—C7	2.0 (5)
Cl1—C1—C6—C5	−178.7 (3)	O1—C7—N2—C8	−0.7 (5)
N4—C9—C10—C11	−179.9 (3)	N1—C7—N2—C8	177.8 (3)
S1—C9—C10—C11	−0.9 (5)	N2—C8—N3—N4	179.0 (3)
C9—C10—C11—C12	177.6 (3)	S1—C8—N3—N4	−0.6 (4)
C10—C11—C12—C17	−171.1 (3)	C10—C9—N4—N3	179.5 (3)
C10—C11—C12—C13	7.9 (6)	S1—C9—N4—N3	0.4 (4)
C17—C12—C13—C14	−0.7 (6)	C8—N3—N4—C9	0.1 (4)

C11—C12—C13—C14	−179.7 (4)	N3—C8—S1—C9	0.7 (3)
C12—C13—C14—C15	0.8 (7)	N2—C8—S1—C9	−178.9 (3)
C13—C14—C15—C16	−0.2 (7)	N4—C9—S1—C8	−0.6 (3)
C14—C15—C16—C17	−0.5 (7)	C10—C9—S1—C8	−179.7 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.93	2.55	3.432 (4)	159
N2—H2A···N3^{ii}	0.82 (4)	2.03 (4)	2.848 (4)	174 (3)

Symmetry codes: (i) −*x*+2, −*y*, −*z*; (ii) −*x*+1, −*y*+2, −*z*.

Fig. 1

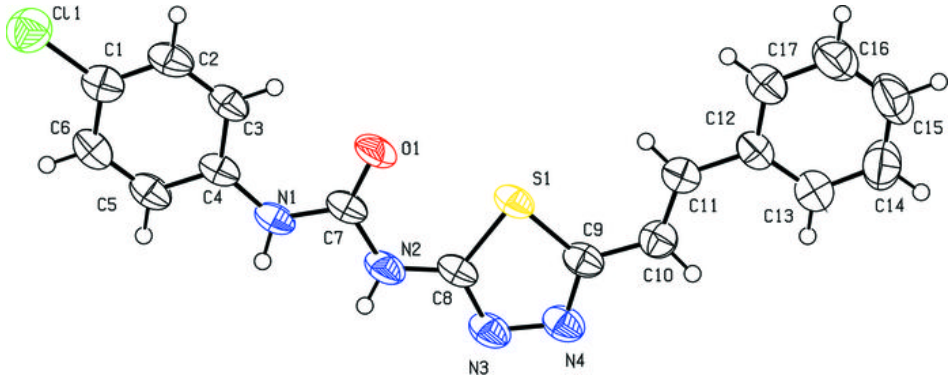
Cl1
C1
C2
C3
C6
C5
C4
N1
C7
O1
N2
S1
C8
C9
C10
C11
C12
C13
C14
C15
C16
C17
N3
N4

Fig. 2