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# 2-(4-Bromophenoxy)-*N*-[5-(*E*)-styryl-1,3,4-thiadiazol-2-yl]acetamide

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**Key indicators**

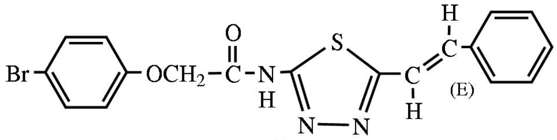
Single-crystal X-ray study
*T* = 292 K
Mean $\sigma$(C–C) = 0.009 Å
*R* factor = 0.068
*wR* factor = 0.185
Data-to-parameter ratio = 17.2

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

In the title compound, $C_{18}H_{14}BrN_3O_2S$, the three rings are nearly coplanar. In the crystal structure, intermolecular N—H···N and C—H···O hydrogen-bond interactions link the molecules into ribbons, displaying alternate rings of graph-set motifs $R_2^2(8)$ and $R_2^2(14)$.

## Comment

1,3,4-Thiadiazole derivatives display significant bioactivities (Wang *et al.*, 1999; Castro & Ball, 1996), and the amide group is an important and representative component of pesticides. In view of our extensive interest, we have prepared a series of 1,3,4-thiadiazole derivatives containing the amide unit. Biological activity tests show that some of them have good activity as plant-growth regulators, including the title compound, (I).



(I)

The molecule of (I) is nearly planar, the dihedral angles formed by the thiadiazole ring with the vinylbenzene and bromobenzene moieties being 4.96 (14) and 5.50 (12)° respectively, and assumes an *E* configuration about the C8═C9 double bond of the vinyl group. Bond distances and angles in (I) are as expected (Table 1). In the crystal structure, intermolecular N—H···N and C—H···O hydrogen-bond interactions occurring between centrosymmetrically related molecules result in the formation of ribbons displaying alternate rings of graph-set motifs $R_2^2(8)$ and $R_2^2(14)$.

## Experimental

2-Amino-5-styryl-1,3,4-thiadiazole (0.91 g, 4.5 mmol), which was prepared according to a literature method (Lalezari & Shafiee, 1971), acetonitrile (15 ml) and triethylamine (4.2 ml) were placed in a dried round-bottomed flask. Then 4-bromophenoxyacetic acid chloride (1.12 g, 4.5 mmol; obtained commercially and used without further purification), obtained in 91% yield by refluxing 4-bromophenoxyacetic acid and an excess of thionyl chloride, was added dropwise, with cooling and stirring. The mixture was stirred at about 340 K for a further 3 h. The solvent was evaporated, and the residue was suspended in water. The solid was removed by filtration, dried and recrystallized from ethanol and DMF (1:1) to give (I) (87% yield). Suitable crystals for the X-ray analysis were obtained by slow evaporation of a methanol–DMF (1:3) solution at room temperature (m.p. 525–526 K). Elemental analysis: Analysis calculated for $C_{18}H_{14}BrN_3O_2S$: C 51.93, H 3.39, N 10.09%; found: C 51.87, H 3.43, N 10.12%.

*Crystal data*

$C_{18}H_{14}BrN_3O_2S$
$M_r$ = 416.29
Triclinic, $P\overline{1}$
$a$ = 5.1151 (9) Å
$b$ = 9.5790 (18) Å
$c$ = 18.426 (3) Å
$\alpha$ = 87.292 (3)°
$\beta$ = 83.782 (3)°
$\gamma$ = 87.021 (4)°
$V$ = 895.5 (3) Å$^3$

$Z$ = 2
$D_x$ = 1.544 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 1434 reflections
$\theta$ = 2.4–19.8°
$\mu$ = 2.43 mm$^{-1}$
$T$ = 292 (1) K
Plate, colourless
0.40 × 0.16 × 0.04 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.443, $T_{\max}$ = 0.909
10201 measured reflections

3898 independent reflections
1930 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.119
$\theta_{\max}$ = 27.0°
$h = -6 \rightarrow 6$
$k = -12 \rightarrow 12$
$l = -23 \rightarrow 23$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.185$
$S$ = 0.97
3898 reflections
226 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 0.50 e Å$^{-3}$
$\Delta\rho_{\min}$ = −0.38 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C6—C7 | 1.454 (7) | C9—S1 | 1.741 (5) |
| C7—C8 | 1.327 (7) | C10—N2 | 1.303 (6) |
| C8—C9 | 1.446 (7) | C10—S1 | 1.711 (5) |
| C9—N1 | 1.310 (6) | N1—N2 | 1.373 (5) |
| | | | |
| C8—C7—C6 | 126.8 (6) | N2—C10—S1 | 114.6 (4) |
| C7—C8—C9 | 125.5 (5) | O1—C11—N3 | 122.2 (5) |
| N1—C9—S1 | 113.6 (4) | C10—S1—C9 | 86.8 (2) |
| | | | |
| C1—C6—C7—C8 | −3.0 (10) | S1—C10—N3—C11 | −1.9 (7) |
| C6—C7—C8—C9 | 177.3 (5) | C14—C13—O2—C12 | −176.7 (5) |
| C7—C8—C9—N1 | −175.0 (6) | C11—C12—O2—C13 | −172.2 (4) |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3$A$···N2$^{\rm i}$ | 0.86 | 2.02 | 2.869 (6) | 171 |
| C14—H14···O1$^{\rm ii}$ | 0.93 | 2.42 | 3.086 (6) | 128 |

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

All H atoms were placed in geometrically idealized positions (C—H = 0.93–0.97 Å; N—H = 0.86 Å) and constrained to ride on their parent atoms, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C,N). The $R_{\rm int}$ value is rather high, perhaps because the crystal is so thin that the equivalent diffraction intensities measured in different directions are evidently inequal.

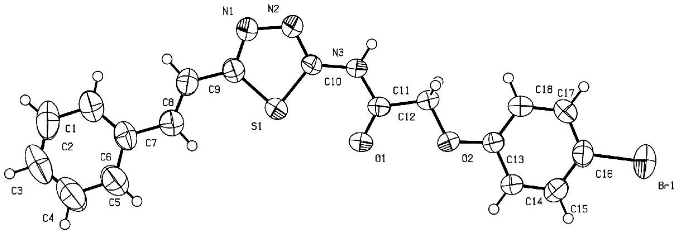


**Figure 1**
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

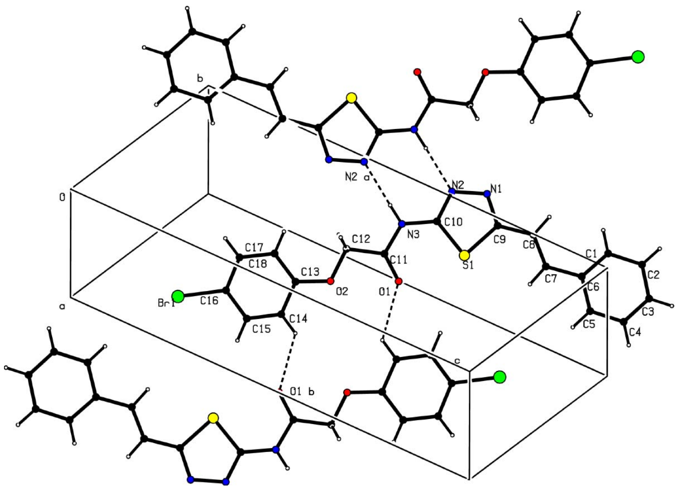


**Figure 2**
Packing diagram of (I) [symmetry codes: (a) $-x, 2-y, 1-z$; (b) $2-x, 1-y, 1-z$]. Hydrogen-bond interactions are shown as dashed lines.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-NT* (Siemens, 1995); software used to prepare material for publication: *SHELXTL-NT*.

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