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# 2-(5-Bromothiophene-2-sulfonamido)benzoic acid

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In the title molecule, $C_{11}H_8BrO_4S_2$, all bond lengths and angles are within normal ranges. Strong intermolecular O—H$\cdots$O interactions link the molecules into centrosymmetric dimers.

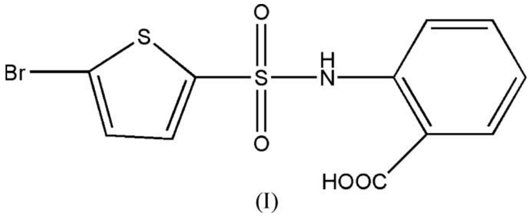
**Key indicators**

Single-crystal X-ray study
$T$ = 298 K
Mean $\sigma$(C–C) = 0.004 Å
$R$ factor = 0.031
$wR$ factor = 0.081
Data-to-parameter ratio = 12.8

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

## Comment

The sulfonamide group is present in many bioactive compounds and may be used as a protecting group (Zhang *et al.*, 2006; Yu, 2006). Many sulfonamide derivatives have been synthesized, examples being *N*-*tert*-butyl-4-toluenesulfonamide (Zhang *et al.*, 2006), *N*-benzyl-5-[*N*-benzyl-*N*-(*tert*-butyloxycarbonyl)amino]-*N*-(*tert*-butyloxycarbonyl)-1,3,4-thiadiazol-2-sulfonamide (Camí *et al.*, 2000) and *N*-cyclohexyl-4-methylbenzenesulfonamide (Yu, 2006). We report here the synthesis and crystal structure of the title compound, (I).



(I)

The bond lengths and angles in (I) (Fig. 1) are within normal ranges (Allen *et al.*, 1987) and comparable with those reported in previous similar studies (Kazak *et al.*, 2000). The benzene and thiophene groups make a dihedral angle of 88.64 (15)°. In the crystal structure, strong intermolecular O—H$\cdots$O interactions generate an $R_2^2(8)$ graph-set motif (Bernstein *et al.*, 1995).

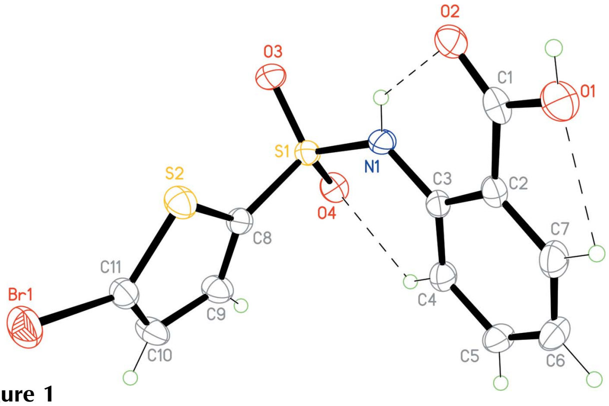


**Figure 1**
The structure of (I), showing the atom numbering and displacement ellipsoids drawn at the 30% probability level. Intramolecular hydrogen bonds are shown as dashed lines.

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## Experimental

5-Bromothiophene-2-sulfonyl chloride (5 mmol, 1.304 g), 2-aminobenzoic acid (5 mmol, 0.685 g) and *N*,*N*-dimethylpyridin-4-amine (DMAP) (0.5 mmol, 0.061 g) were added to acetone (15 ml) at room temperature with stirring. The reaction was allowed to proceed for 48 h at room temperature, followed by column chromatographic separation. The purified product was dissoved in ethanol–acetone **(ratio?)**, and allowed to stand for approximately 15 d until single crystals formed.

*Crystal data*

$C_{11}H_8BrNO_4S_2$
$M_r = 362.21$
Monoclinic, $C2/c$
$a = 28.064$ (2) Å
$b = 8.7216$ (7) Å
$c = 10.7416$ (9) Å
$\beta = 100.9320$ (10)°
$V = 2581.5$ (4) Å$^3$
$Z = 8$
$D_x = 1.864$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu = 3.52$ mm$^{-1}$
$T = 298$ (2) K
Block, colourless
0.28 × 0.23 × 0.16 mm

*Data collection*

Bruker APEX area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.401$, $T_{\max} = 0.576$
6547 measured reflections
2287 independent reflections
1878 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$
$\theta_{\max} = 25.0°$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.081$
$S = 1.04$
2287 reflections
178 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.037P)^2 + 2.6357P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.32$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.28$ e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Br1—C11 | 1.864 (3) | S2—C11 | 1.709 (3) |
| S1—O4 | 1.424 (2) | S2—C8 | 1.723 (3) |
| S1—N1 | 1.620 (2) | O1—C1 | 1.317 (3) |
| S1—C8 | 1.738 (3) | | |
| C11—S2—C8 | 90.24 (14) | C10—C11—S2 | 113.4 (2) |
| C9—C8—S2 | 111.8 (2) | | |

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C5—H5···O3$^{\rm i}$ | 0.93 | 2.50 | 3.387 (4) | 159 |
| C7—H7···O1 | 0.93 | 2.35 | 2.694 (4) | 101 |
| C4—H4···O4 | 0.93 | 2.38 | 3.039 (4) | 128 |
| N1—H1···O2 | 0.823 (18) | 1.99 (3) | 2.644 (3) | 136 (3) |
| O1—H1*A*···O2$^{\rm ii}$ | 0.792 (18) | 1.934 (19) | 2.716 (3) | 169 (4) |

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

The H atoms on N1 and O1 were located in a difference Fourier map and refined isotropically. All other H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of C$sp^2$—H = 0.93 Å, with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(parent atom).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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, 2002); software used to prepare material for publication: *SHELXL97*.

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