# 2-[(3-Bromoanilino)methyl]-1,2-benzo-thiazol-3(2H)-one

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The title compound, $C_{14}H_{11}BrN_2OS$, was synthesized by the reaction of 1,2-benzothiazol-3(2H)-one with formalin and 3-bromoaniline in ethanol. The 1,2-benzothiazolone ring system is approximately planar [maximum deviation = 0.0142 **(s.u.?)** Å] and forms a dihedral angle of 79.19 (5)° with the benzene ring. In the crystal, molecules are linked by N—H···O, C—H···O and C—H···Br interactions.

## Related literature

For background to the synthesis of benzoisothiazolone derivatives, see: Davis (1972); Elgazwy & Abdel-Sattar (2003). For the biological activity of 1,2-benzoisothiazolone derivatives, see: Taubert *et al.* (2002). For structural studies of related alkyl 3-oxo-2,3-dihydro-1,2-benzothiazole-2-carboxylate derivatives, see: Wang *et al.* (2011); Wang, Yang *et al.* (2011a,b).
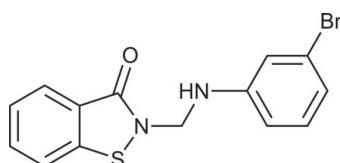


## Experimental

### Crystal data

| | |
|---|---|
| $C_{14}H_{11}BrN_2OS$ | Monoclinic, $P2_1/c$ |
| $M_r = 335.22$ | $a = 7.351$ (2) Å |
| $b = 22.781$ (7) Å | Mo $K\alpha$ radiation |
| $c = 8.559$ (3) Å | $\mu = 3.19$ mm$^{-1}$ |
| $\beta = 109.580$ (4)° | $T = 153$ K |
| $V = 1350.5$ (7) Å$^3$ | $0.38 \times 0.37 \times 0.31$ mm |
| $Z = 4$ | |

### Data collection

| | |
|---|---|
| Rigaku AFC10/Saturn724+ diffractometer | 11631 measured reflections |
| Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) | 3587 independent reflections |
| | 2709 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.374$, $T_{max} = 0.436$ | $R_{int} = 0.037$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.032$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.069$ | |
| $S = 1.00$ | |
| 3587 reflections | $\Delta\rho_{max} = 0.44$ e Å$^{-3}$ |
| 176 parameters | $\Delta\rho_{min} = -0.52$ e Å$^{-3}$ |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$N$···O1$^i$ | 0.82 (2) | 2.14 (2) | 2.939 (2) | 167 (2) |
| C3—H3···O1$^{ii}$ | 0.95 | 2.59 | 3.484 (3) | 157 |
| C10—H10···Br1$^{iii}$ | 0.95 | 2.93 | 3.545 (3) | 124 |
| C14—H14···O1$^i$ | 0.95 | 2.46 | 3.207 (3) | 135 |

Symmetry codes: (i) $-x + 2, -y + 1, -z + 2$; (ii) $x, y, z + 1$; (iii) $x + 1, -y + \frac{3}{2}, z + \frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* and *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2723).

## References

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# 2-[(3-Bromoanilino)methyl]-1,2-benzothiazol-3(2*H*)-one

## Xiang-Hui Wang, Jian-Xin Yang, Qiang Lin and Jun-Hua Chen

## Comment

The work presented herein is part of our interest in synthesizing various benzisothiazolone derivatives and confirming their structures by X-ray analysis (Wang *et al.*, 2011; Wang, Yang *et al.*, 2011*a*,*b*). These compounds will be utilized for the study of comparative bioactivity.

The molecular structure of the title compound is shown in Fig. 1. In the molecule, the benzisothiazolone ring system is approximately planar with a maximum deviation from the mean plane of 0.0142 A ° for the atom C1, and the dihedral angle between the benzene ring and the benzisothiazolone ring is 79.169 (5)°. In the crystal structure, intermolecular N—H···O, C—H···O and C—H···Br hydrogen bonds (Table 1) link molecules into a three-dimensional network (Fig. 2).

## Experimental

An ethanol solution (20 ml) containing 1,2-benzothiazol-3(2*H*)-one (1.51 g, 0.01 mol), formalin (1 mL) and 3-bromo-aniline (1.72 g, 0.01 mol) was stirred at room temperature for 4.5 h to afford the title compound (1.97 g, yield 58.8%). Single crystals suitable for X-ray measurements were obtained by recrystallization of the title compound from trichloro-methane/methanol (1:1 *v*/*v*) at room temperature.

## Refinement

The amine H atom was located in a difference Fourier map and refined freely. All other H atoms were placed at calculated positions and refined in riding mode, with C—H = 0.95–0.99 Å. The $U_{iso}$(H) values were constrained to be 1.5$U_{eq}$(C) for the methyl H atoms or 1.2$U_{eq}$(C) for the remaining H atoms.

## Computing details

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear* (Rigaku, 2008); data reduction: *CrystalClear* (Rigaku, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).
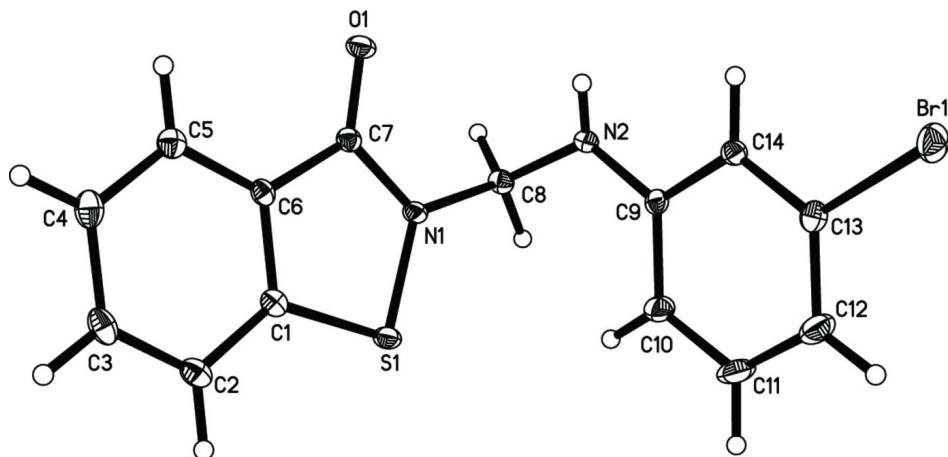
**Figure 1**

The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level. H atoms are presented as small spheres of arbitrary radius.
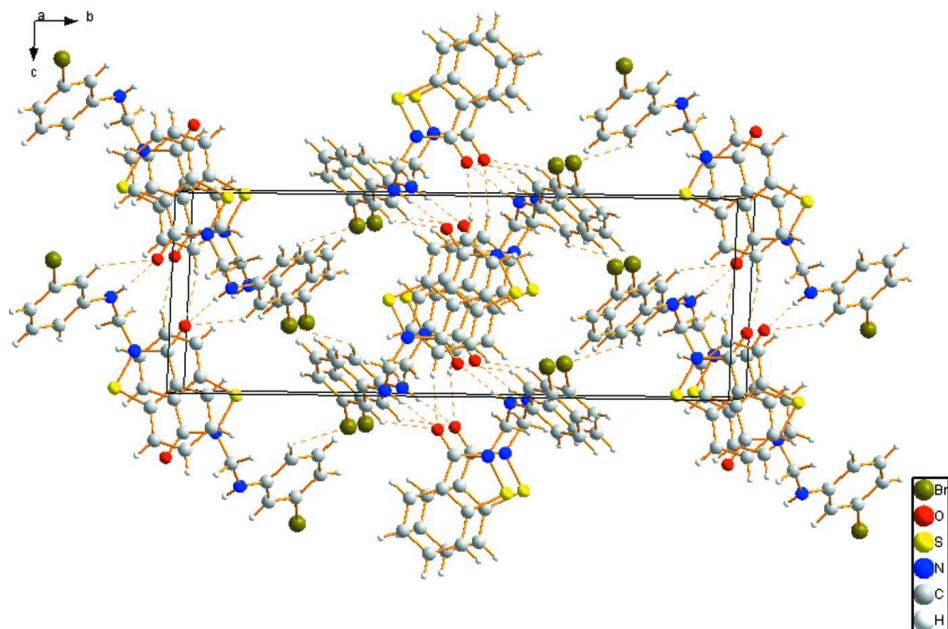


**Figure 2**

A view of the C—H⋯O and C—H⋯Br interactions (dashed lines) in the crystal structure of the title compound.

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*Crystal data*

| | |
|---|---|
| $C_{14}H_{11}BrN_2OS$ | $V = 1350.5$ (7) Å$^3$ |
| $M_r = 335.22$ | $Z = 4$ |
| Monoclinic, $P2_1/c$ | $F(000) = 672$ |
| Hall symbol: -P 2ybc | $D_x = 1.649$ Mg m$^{-3}$ |
| $a = 7.351$ (2) Å | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $b = 22.781$ (7) Å | Cell parameters from 4184 reflections |
| $c = 8.559$ (3) Å | $\theta = 2.7–29.1°$ |
| $\beta = 109.580$ (4)° | $\mu = 3.19$ mm$^{-1}$ |

$T = 153$ K

Block, colourless

$0.38 × 0.37 × 0.31$ mm

*Data collection*

| | |
|---|---|
| Rigaku AFC10/Saturn724+ diffractometer | 11631 measured reflections |
| Radiation source: Rotating Anode | 3587 independent reflections |
| Graphite monochromator | 2709 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 28.5714 pixels mm$^{-1}$ | $R_{int} = 0.037$ |
| phi and $\omega$ scans | $\theta_{max} = 29.1°$, $\theta_{min} = 2.7°$ |
| Absorption correction: multi-scan | $h = -10\rightarrow9$ |
| (*ABSCOR*; Higashi, 1995) | $k = -31\rightarrow30$ |
| | $l = -11\rightarrow11$ |

$T_{min} = 0.374$, $T_{max} = 0.436$

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.032$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.069$ | |
| $S = 1.00$ | H atoms treated by a mixture of independent and constrained refinement |
| 3587 reflections | |
| 176 parameters | $w = 1/[\sigma^2(F_o^2) + (0.0289P)^2 + 0.160P]$ |
| 0 restraints | where $P = (F_o^2 + 2F_c^2)/3$ |
| Primary atom site location: structure-invariant direct methods | $(\Delta/\sigma)_{max} < 0.001$ |
| | $\Delta\rho_{max} = 0.44$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.52$ 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.37553 (3) | 0.693276 (11) | 0.83530 (3) | 0.03101 (8) |
| O1 | 1.1959 (2) | 0.47887 (6) | 1.16801 (16) | 0.0223 (3) |
| S1 | 1.30876 (8) | 0.60263 (2) | 1.48237 (6) | 0.02068 (12) |
| N1 | 1.2660 (2) | 0.56804 (7) | 1.29651 (19) | 0.0181 (4) |
| C13 | 0.6410 (3) | 0.69583 (9) | 0.9710 (3) | 0.0220 (4) |
| C7 | 1.2302 (3) | 0.50892 (9) | 1.2939 (2) | 0.0174 (4) |
| N2 | 1.0771 (2) | 0.60956 (8) | 1.0275 (2) | 0.0184 (4) |
| C5 | 1.2107 (3) | 0.43397 (10) | 1.5099 (3) | 0.0218 (4) |
| H5 | 1.1821 | 0.4025 | 1.4327 | 0.026* |
| C3 | 1.2648 (3) | 0.47107 (10) | 1.7852 (3) | 0.0253 (5) |
| H3 | 1.2716 | 0.4638 | 1.8963 | 0.030* |
| C1 | 1.2822 (3) | 0.53648 (9) | 1.5741 (2) | 0.0181 (4) |
| C9 | 0.9559 (3) | 0.65290 (9) | 1.0506 (2) | 0.0172 (4) |

| C10 | 1.0203 (3) | 0.69745 (9) | 1.1676 (3) | 0.0261 (5) |
| H10 | 1.1519 | 0.6985 | 1.2368 | 0.031* |
| C14 | 0.7614 (3) | 0.65249 (9) | 0.9498 (2) | 0.0182 (4) |
| H14 | 0.7134 | 0.6229 | 0.8682 | 0.022* |
| C6 | 1.2401 (3) | 0.49047 (9) | 1.4604 (2) | 0.0168 (4) |
| C8 | 1.2648 (3) | 0.59860 (9) | 1.1440 (2) | 0.0184 (4) |
| H8A | 1.3328 | 0.6366 | 1.1755 | 0.022* |
| H8B | 1.3384 | 0.5747 | 1.0891 | 0.022* |
| C2 | 1.2955 (3) | 0.52715 (10) | 1.7396 (3) | 0.0237 (5) |
| H2 | 1.3246 | 0.5584 | 1.8174 | 0.028* |
| C4 | 1.2239 (3) | 0.42447 (10) | 1.6723 (3) | 0.0259 (5) |
| H4 | 1.2051 | 0.3861 | 1.7078 | 0.031* |
| C12 | 0.7015 (3) | 0.74034 (11) | 1.0860 (3) | 0.0324 (5) |
| H12 | 0.6149 | 0.7697 | 1.0973 | 0.039* |
| C11 | 0.8935 (4) | 0.74030 (11) | 1.1840 (3) | 0.0349 (6) |
| H11 | 0.9402 | 0.7703 | 1.2645 | 0.042* |
| H2N | 1.017 (3) | 0.5816 (10) | 0.975 (3) | 0.023 (6)* |

*Atomic displacement parameters (Å²)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.02204 (12) | 0.03134 (14) | 0.03771 (15) | 0.00613 (10) | 0.00744 (9) | 0.00158 (11) |
| O1 | 0.0263 (8) | 0.0235 (8) | 0.0165 (8) | −0.0016 (7) | 0.0064 (6) | −0.0054 (6) |
| S1 | 0.0272 (3) | 0.0200 (3) | 0.0155 (3) | −0.0026 (2) | 0.0080 (2) | −0.0035 (2) |
| N1 | 0.0253 (9) | 0.0177 (9) | 0.0124 (9) | −0.0007 (7) | 0.0076 (7) | −0.0009 (7) |
| C13 | 0.0227 (10) | 0.0203 (11) | 0.0235 (12) | 0.0014 (9) | 0.0083 (9) | 0.0035 (9) |
| C7 | 0.0150 (9) | 0.0194 (11) | 0.0166 (11) | 0.0010 (8) | 0.0038 (8) | −0.0013 (8) |
| N2 | 0.0189 (9) | 0.0179 (9) | 0.0162 (9) | 0.0000 (7) | 0.0029 (7) | −0.0024 (7) |
| C5 | 0.0182 (10) | 0.0234 (11) | 0.0229 (12) | 0.0000 (9) | 0.0059 (8) | 0.0005 (9) |
| C3 | 0.0220 (11) | 0.0365 (13) | 0.0191 (12) | 0.0016 (10) | 0.0092 (9) | 0.0068 (10) |
| C1 | 0.0137 (9) | 0.0231 (11) | 0.0178 (11) | −0.0009 (8) | 0.0054 (8) | 0.0001 (8) |
| C9 | 0.0207 (10) | 0.0151 (10) | 0.0164 (10) | 0.0000 (8) | 0.0071 (8) | 0.0024 (8) |
| C10 | 0.0239 (11) | 0.0211 (11) | 0.0289 (13) | −0.0026 (10) | 0.0032 (9) | −0.0066 (9) |
| C14 | 0.0228 (11) | 0.0176 (10) | 0.0150 (11) | −0.0001 (8) | 0.0073 (8) | 0.0006 (8) |
| C6 | 0.0128 (9) | 0.0212 (10) | 0.0155 (10) | 0.0019 (8) | 0.0038 (7) | 0.0014 (8) |
| C8 | 0.0208 (10) | 0.0215 (11) | 0.0154 (10) | −0.0010 (9) | 0.0095 (8) | 0.0005 (8) |
| C2 | 0.0229 (11) | 0.0314 (13) | 0.0177 (11) | 0.0002 (9) | 0.0079 (9) | −0.0016 (9) |
| C4 | 0.0232 (11) | 0.0277 (12) | 0.0279 (13) | 0.0004 (10) | 0.0098 (9) | 0.0081 (10) |
| C12 | 0.0337 (13) | 0.0256 (12) | 0.0389 (14) | 0.0061 (11) | 0.0134 (11) | −0.0091 (11) |
| C11 | 0.0392 (14) | 0.0251 (13) | 0.0382 (14) | −0.0003 (11) | 0.0100 (11) | −0.0165 (11) |

*Geometric parameters (Å, º)*

| Br1—C13 | 1.908 (2) | C3—C4 | 1.398 (3) |
|---|---|---|---|
| O1—C7 | 1.229 (2) | C3—H3 | 0.9500 |
| S1—N1 | 1.7074 (17) | C1—C6 | 1.393 (3) |
| S1—C1 | 1.740 (2) | C1—C2 | 1.403 (3) |
| N1—C7 | 1.371 (3) | C9—C10 | 1.393 (3) |
| N1—C8 | 1.476 (2) | C9—C14 | 1.401 (3) |
| C13—C14 | 1.378 (3) | C10—C11 | 1.389 (3) |

| | | | |
|---|---|---|---|
| C13—C12 | 1.379 (3) | C10—H10 | 0.9500 |
| C7—C6 | 1.464 (3) | C14—H14 | 0.9500 |
| N2—C9 | 1.388 (3) | C8—H8A | 0.9900 |
| N2—C8 | 1.427 (2) | C8—H8B | 0.9900 |
| N2—H2N | 0.82 (2) | C2—H2 | 0.9500 |
| C5—C4 | 1.378 (3) | C4—H4 | 0.9500 |
| C5—C6 | 1.394 (3) | C12—C11 | 1.379 (3) |
| C5—H5 | 0.9500 | C12—H12 | 0.9500 |
| C3—C2 | 1.376 (3) | C11—H11 | 0.9500 |
| | | | |
| N1—S1—C1 | 90.41 (9) | C11—C10—H10 | 119.8 |
| C7—N1—C8 | 120.30 (16) | C9—C10—H10 | 119.8 |
| C7—N1—S1 | 116.28 (13) | C13—C14—C9 | 118.83 (19) |
| C8—N1—S1 | 123.42 (13) | C13—C14—H14 | 120.6 |
| C14—C13—C12 | 123.6 (2) | C9—C14—H14 | 120.6 |
| C14—C13—Br1 | 117.97 (16) | C1—C6—C5 | 120.22 (18) |
| C12—C13—Br1 | 118.46 (17) | C1—C6—C7 | 113.01 (18) |
| O1—C7—N1 | 122.90 (18) | C5—C6—C7 | 126.76 (18) |
| O1—C7—C6 | 128.46 (19) | N2—C8—N1 | 114.72 (16) |
| N1—C7—C6 | 108.64 (17) | N2—C8—H8A | 108.6 |
| C9—N2—C8 | 122.78 (18) | N1—C8—H8A | 108.6 |
| C9—N2—H2N | 112.0 (16) | N2—C8—H8B | 108.6 |
| C8—N2—H2N | 117.8 (16) | N1—C8—H8B | 108.6 |
| C4—C5—C6 | 119.1 (2) | H8A—C8—H8B | 107.6 |
| C4—C5—H5 | 120.5 | C3—C2—C1 | 117.7 (2) |
| C6—C5—H5 | 120.5 | C3—C2—H2 | 121.2 |
| C2—C3—C4 | 121.8 (2) | C1—C2—H2 | 121.2 |
| C2—C3—H3 | 119.1 | C5—C4—C3 | 120.3 (2) |
| C4—C3—H3 | 119.1 | C5—C4—H4 | 119.9 |
| C6—C1—C2 | 121.0 (2) | C3—C4—H4 | 119.9 |
| C6—C1—S1 | 111.65 (15) | C13—C12—C11 | 116.9 (2) |
| C2—C1—S1 | 127.33 (17) | C13—C12—H12 | 121.5 |
| N2—C9—C10 | 122.76 (19) | C11—C12—H12 | 121.5 |
| N2—C9—C14 | 118.63 (19) | C12—C11—C10 | 121.6 (2) |
| C10—C9—C14 | 118.60 (19) | C12—C11—H11 | 119.2 |
| C11—C10—C9 | 120.5 (2) | C10—C11—H11 | 119.2 |
| | | | |
| C1—S1—N1—C7 | 0.55 (16) | S1—C1—C6—C7 | 0.5 (2) |
| C1—S1—N1—C8 | −179.97 (16) | C4—C5—C6—C1 | 0.1 (3) |
| C8—N1—C7—O1 | 0.0 (3) | C4—C5—C6—C7 | −179.39 (19) |
| S1—N1—C7—O1 | 179.45 (15) | O1—C7—C6—C1 | −179.89 (19) |
| C8—N1—C7—C6 | −179.87 (16) | N1—C7—C6—C1 | −0.1 (2) |
| S1—N1—C7—C6 | −0.4 (2) | O1—C7—C6—C5 | −0.4 (3) |
| N1—S1—C1—C6 | −0.57 (15) | N1—C7—C6—C5 | 179.41 (18) |
| N1—S1—C1—C2 | −179.34 (19) | C9—N2—C8—N1 | 74.6 (2) |
| C8—N2—C9—C10 | 14.7 (3) | C7—N1—C8—N2 | 76.3 (2) |
| C8—N2—C9—C14 | −166.54 (18) | S1—N1—C8—N2 | −103.16 (19) |
| N2—C9—C10—C11 | 179.0 (2) | C4—C3—C2—C1 | 0.7 (3) |
| C14—C9—C10—C11 | 0.3 (3) | C6—C1—C2—C3 | −0.2 (3) |

| C12—C13—C14—C9 | 0.5 (3) | S1—C1—C2—C3 | 178.47 (16) |
|---|---|---|---|
| Br1—C13—C14—C9 | −178.70 (15) | C6—C5—C4—C3 | 0.4 (3) |
| N2—C9—C14—C13 | −179.28 (18) | C2—C3—C4—C5 | −0.9 (3) |
| C10—C9—C14—C13 | −0.5 (3) | C14—C13—C12—C11 | −0.3 (4) |
| C2—C1—C6—C5 | −0.2 (3) | Br1—C13—C12—C11 | 178.94 (18) |
| S1—C1—C6—C5 | −179.05 (15) | C13—C12—C11—C10 | 0.0 (4) |
| C2—C1—C6—C7 | 179.34 (18) | C9—C10—C11—C12 | 0.0 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*N*···O1[i] | 0.82 (2) | 2.14 (2) | 2.939 (2) | 167 (2) |
| C3—H3···O1[ii] | 0.95 | 2.59 | 3.484 (3) | 157 |
| C10—H10···Br1[iii] | 0.95 | 2.93 | 3.545 (3) | 124 |
| C14—H14···O1[i] | 0.95 | 2.46 | 3.207 (3) | 135 |

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+2; (ii) *x*, *y*, *z*+1; (iii) *x*+1, −*y*+3/2, *z*+1/2.