# 3-Benzoyl-1-(2-methoxyphenyl)thiourea

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In the title compound, $C_{15}H_{14}N_2O_2S$, the central $C_2N_2OS$ moiety is planar (r.m.s. deviation of fitted atoms = 0.0336 Å). This is ascribed to the formation of an $S(6)$ loop stabilized by an intramolecular N—H⋯O hydrogen bond; additional intramolecular N—H⋯O and C—H⋯S contacts are also noted. The dihedral angles between the central unit and the phenyl and benzene rings are 23.79 (7) and 29.52 (5)°, respectively. The thione S and ketone O atoms are mutually *anti*, as are the N—H H atoms; the O atoms lie to the same side of the molecule. Centrosymmetric eight-membered {⋯HNC=S}₂ synthons feature in the crystal packing. The resulting inversion dimers stack along the *a* axis and are connected into a three-dimensional structure by C—H⋯O and C—H⋯$\pi$ interactions.

## Related literature

For complexation of *N*-benzoyl-*N'*-arylthiourea derivatives to transition metals, see: Selvakumaran *et al.* (2011). For the structure of the unsubstituted parent compound, see: Yamin & Yusof (2003).
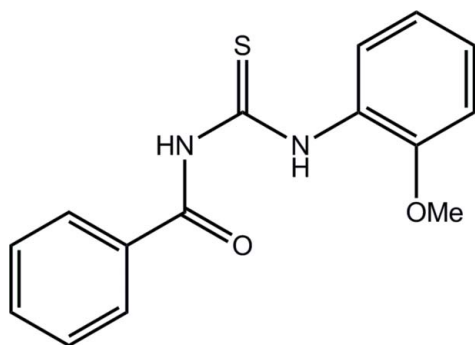


## Experimental

### Crystal data

| | |
|---|---|
| $C_{15}H_{14}N_2O_2S$ | $V = 1379.76$ (4) Å³ |
| $M_r = 286.34$ | $Z = 4$ |
| Monoclinic, $P2_1/c$ | Cu $K\alpha$ radiation |
| $a = 5.9358$ (1) Å | $\mu = 2.11$ mm⁻¹ |
| $b = 25.6916$ (4) Å | $T = 100$ K |
| $c = 9.0535$ (1) Å | $0.30 \times 0.25 \times 0.20$ mm |
| $\beta = 92.065$ (1)° | |

### Data collection

| | |
|---|---|
| Agilent SuperNova Dual diffractometer with an Atlas detector | 5143 measured reflections |
| | 2721 independent reflections |
| | 2505 reflections with $I > 2\sigma(I)$ |
| Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012) $T_{min} = 0.467$, $T_{max} = 1.000$ | $R_{int} = 0.016$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.034$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.097$ | |
| $S = 1.04$ | |
| 2721 reflections | $\Delta\rho_{max} = 0.27$ e Å⁻³ |
| 189 parameters | $\Delta\rho_{min} = -0.40$ e Å⁻³ |

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

$Cg1$ is the centroid of the C9–C14 benzene ring.

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| N2—H2n⋯O1 | 0.905 (18) | 1.867 (18) | 2.6316 (15) | 141.0 (16) |
| C10—H10⋯S1 | 0.95 | 2.68 | 3.2241 (13) | 117 |
| N2—H2n⋯O2 | 0.90 (2) | 2.231 (19) | 2.5819 (15) | 102.5 (14) |
| N1—H1n⋯S1ⁱ | 0.902 (18) | 2.636 (18) | 3.4976 (12) | 160.1 (15) |
| C15—H15B⋯O1ⁱⁱ | 0.98 | 2.57 | 3.4273 (19) | 146 |
| C15—H15C⋯Cg1ⁱⁱⁱ | 0.98 | 2.81 | 3.6248 (17) | 141 |

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2519).

## References

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# supporting information

## 3-Benzoyl-1-(2-methoxyphenyl)thiourea

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### S1. Comment

*N*-Benzoyl-*N′*-arylthiourea derivatives, of which the title compound is an example are versatile ligands with coordination possible *via* the S, O or N atom, and various combinations of these. The title compound was prepared in connection with on-going studies involving complexation of *N*-benzoyl-*N′*-arylthiourea derivatives to transition metals, *e.g.* Pd$^{II}$ (Selvakumaran *et al.*, 2011).

In the title compound, Fig. 1, the thione and ketone atoms are *anti* with respect to each other. Similarly, the N—H H-atoms are *anti* to each other, and the oxygen atoms lie to the same side of the molecule. The central chromophore is planar with a r.m.s. deviation of 0.0336 Å [maximum deviations of 0.0449 (5) Å for S1, and -0.0460 (9) Å for N1] owing to the presence of an intramolecular N—H⋯O hydrogen bond which closes an *S*(6) loop (Table 1). Weaker intramolecular N—H⋯O and C—H⋯S contacts are also noted (Table 1). Despite this, a significant twist is evident in the molecule as manifested in the dihedral angle of 53.06 (5)° between the six-membered rings. The relative orientation of the atoms and deviations from planarity described above mimic those reported for the unsubstituted parent compound, PhC(═O)N(H)C(═S)N(H)Ph where the dihedral angle between the phenyl rings is 33.26 (6)° (Yamin & Yusof, 2003).

The most significant interaction in the crystal packing is the formation of centrosymmetric eight-membered {⋯HNC=S}$_2$ synthons owing to the presence of N—H⋯S hydrogen bonds (Table ). These inversion dimers stack along the *a* axis and are connected into a three-dimensional architecture by C—H⋯O and C—H⋯π interactions (Fig. 2 and Table 1).

### S2. Experimental

A solution of benzoyl chloride (0.005 mol, 0.7029 g) in acetone (30 ml) was added drop wise to a suspension of potassium thiocyanate (0.005 mol, 0.4859 g) in anhydrous acetone (30 ml). The reaction mixture was heated under reflux for 45 minutes and then cooled to room temperature. A solution of substituted 2-methoxyaniline (0.005 mol, 0.6158 g). in acetone (30 ml) was added and the resulting mixture was stirred for 2 h. Hydrochloric acid (0.1 N, 300 ml) was added and resulting solid was filtered, washed with water and dried *in vacuo*. The resulting solid product was recrystallized from ethanol/dichloromethane (1:2 ratio) solution. Yield: 87%, *M*. pt: 409 K. Anal. Calcd. for C$_{15}$H$_{14}$N$_2$O$_2$S (%): C, 62.9; H, 4.9; N, 9.8; Found: C, 63.1; H, 5.1; N, 9.6. Spectroscopic data for the title compound are given in the archived CIF.

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H = 0.95 to 0.98 Å, $U_{iso}$(H) = 1.2U$_{eq}$(C) or 1.5$U_{eq}$(C$_{methyl}$)] and were included in the refinement in the riding model approximation. The N-bound H-atoms were refined freely.
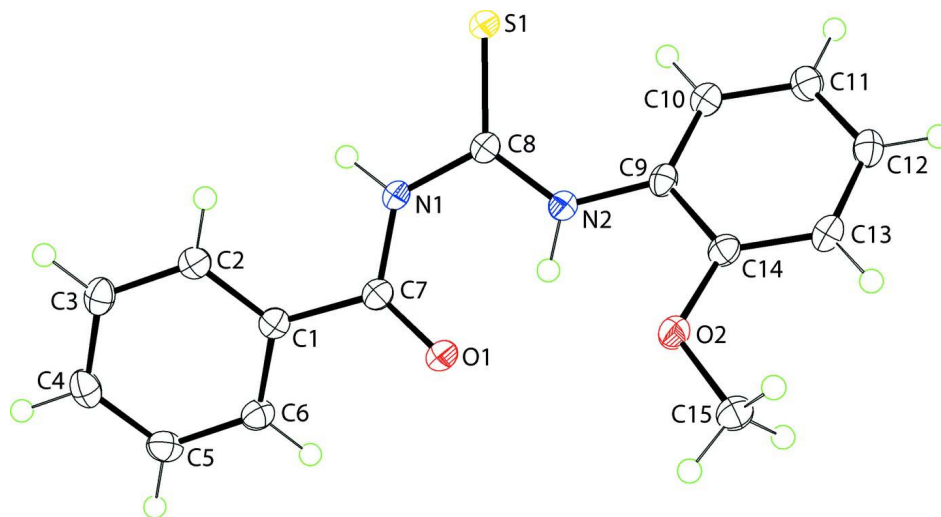
**Figure 1**

Molecular structure of the title molecule, showing the atom-labelling. Displacement ellipsoids are drawn at the 50% probability level.
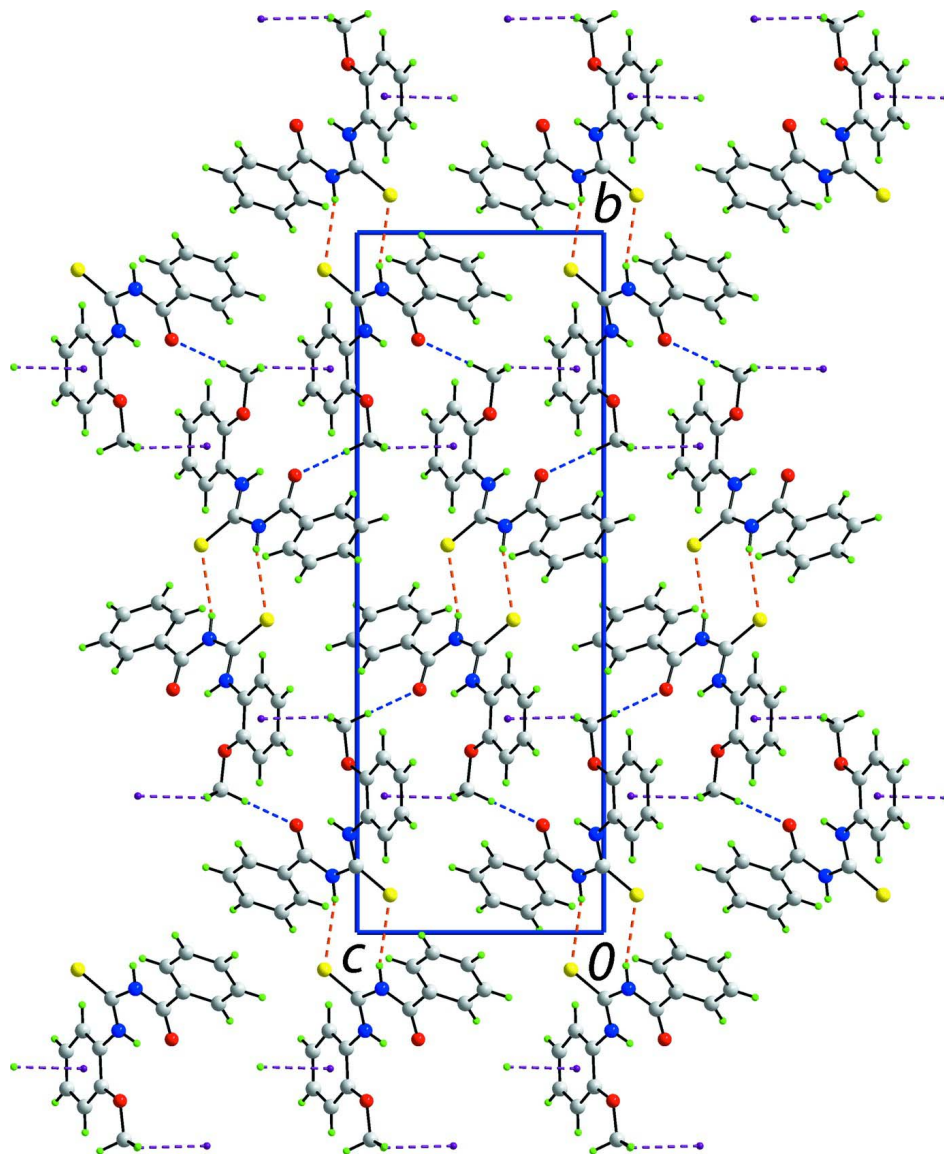
**Figure 2**

A view of the unit-cell contents of the title compound in projection down the *a* axis. The N—H⋯S, C—H⋯O and C—H⋯π interactions are shown as orange, blue and purple dashed lines, respectively.

### 3-Benzoyl-1-(2-methoxyphenyl)thiourea

*Crystal data*

| | |
|---|---|
| $C_{15}H_{14}N_2O_2S$ | $F(000) = 600$ |
| $M_r = 286.34$ | $D_x = 1.378$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 3350 reflections |
| $a = 5.9358$ (1) Å | $\theta = 3.4–74.2°$ |
| $b = 25.6916$ (4) Å | $\mu = 2.11$ mm$^{-1}$ |
| $c = 9.0535$ (1) Å | $T = 100$ K |
| $\beta = 92.065$ (1)° | Block, colourless |
| $V = 1379.76$ (4) Å$^3$ | $0.30 \times 0.25 \times 0.20$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Agilent SuperNova Dual diffractometer with an Atlas detector | $T_{min} = 0.467$, $T_{max} = 1.000$ |
| Radiation source: SuperNova (Cu) X-ray Source | 5143 measured reflections |
| | 2721 independent reflections |
| Mirror monochromator | 2505 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 10.4041 pixels mm$^{-1}$ | $R_{int} = 0.016$ |
| $\omega$ scan | $\theta_{max} = 74.4°$, $\theta_{min} = 3.4°$ |
| Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012) | $h = -7 \rightarrow 6$ |
| | $k = -31 \rightarrow 12$ |
| | $l = -11 \rightarrow 10$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.034$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.097$ | |
| $S = 1.04$ | H atoms treated by a mixture of independent and constrained refinement |
| 2721 reflections | |
| 189 parameters | $w = 1/[\sigma^2(F_o^2) + (0.0671P)^2 + 0.2141P]$ |
| 0 restraints | where $P = (F_o^2 + 2F_c^2)/3$ |
| Primary atom site location: structure-invariant direct methods | $(\Delta/\sigma)_{max} = 0.002$ |
| | $\Delta\rho_{max} = 0.27$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.40$ e Å$^{-3}$ |

*Special details*

**Experimental**. Spectroscopic data for the title compound:
$^1$H NMR (400 MHz, CDCl$_3$, p.p.m.): 3.96 (s, 3H, OCH3); 6.96–7.91 (m, 8H); 8.76 (dd, J = 8.0 Hz & 1.6 Hz, 1H); 9.11 (s, 1H, thiourea NH); 12.85 (s, 1H, amide NH). $^{13}$C NMR (400 MHz, CDCl$_3$, p.p.m.): 56.1; 110.6; 120.2; 123.0; 126.8; 127.2; 127.5; 129.1; 131.1; 133.1; 150.7; 166.5; 176.7. F T—IR (KBr, cm$^{-1}$): 3270 $\nu$(amide N—H), 3014 $\nu$(thiourea N—H), 1672 $\nu$(C=O), 1240 $\nu$(C=S).

**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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.34254 (5) | 0.553335 (12) | 0.63331 (3) | 0.02037 (13) |
| O1 | 0.58134 (17) | 0.65291 (4) | 0.25290 (11) | 0.0228 (2) |
| O2 | 0.30344 (16) | 0.74084 (4) | 0.46245 (11) | 0.0221 (2) |
| N1 | 0.56616 (18) | 0.58059 (4) | 0.39976 (12) | 0.0168 (2) |
| H1n | 0.617 (3) | 0.5477 (7) | 0.410 (2) | 0.025 (4)* |
| N2 | 0.29972 (18) | 0.64037 (4) | 0.46801 (12) | 0.0173 (2) |
| H2n | 0.361 (3) | 0.6586 (7) | 0.394 (2) | 0.034 (5)* |
| C1 | 0.8406 (2) | 0.58513 (5) | 0.20667 (14) | 0.0176 (3) |
| C2 | 0.9874 (2) | 0.54873 (5) | 0.27253 (15) | 0.0190 (3) |
| H2 | 0.9654 | 0.5374 | 0.3709 | 0.023* |

| | | | | |
|------|------------|------------|---------------|-----------|
| C3   | 1.1658 (2) | 0.52905 (5) | 0.19390 (16)  | 0.0217 (3) |
| H3   | 1.2654     | 0.5042      | 0.2385        | 0.026*    |
| C4   | 1.1982 (2) | 0.54569 (5) | 0.05014 (16)  | 0.0236 (3) |
| H4   | 1.3204     | 0.5323      | −0.0032       | 0.028*    |
| C5   | 1.0521 (2) | 0.58180 (5) | −0.01569 (15) | 0.0231 (3) |
| H5   | 1.0740     | 0.5929      | −0.1142       | 0.028*    |
| C6   | 0.8744 (2) | 0.60160 (5) | 0.06219 (15)  | 0.0210 (3) |
| H6   | 0.7754     | 0.6265      | 0.0171        | 0.025*    |
| C7   | 0.6527 (2) | 0.60957 (5) | 0.28644 (14)  | 0.0178 (3) |
| C8   | 0.3977 (2) | 0.59455 (5) | 0.49537 (14)  | 0.0165 (3) |
| C9   | 0.1267 (2) | 0.66553 (5) | 0.54421 (14)  | 0.0173 (3) |
| C10  | −0.0476 (2)| 0.64063 (5) | 0.61365 (14)  | 0.0191 (3) |
| H10  | −0.0534    | 0.6037      | 0.6158        | 0.023*    |
| C11  | −0.2144 (2)| 0.66955 (6) | 0.68032 (15)  | 0.0213 (3) |
| H11  | −0.3336    | 0.6523      | 0.7276        | 0.026*    |
| C12  | −0.2069 (2)| 0.72356 (6) | 0.67787 (16)  | 0.0228 (3) |
| H12  | −0.3192    | 0.7431      | 0.7253        | 0.027*    |
| C13  | −0.0354 (2)| 0.74907 (5) | 0.60610 (15)  | 0.0218 (3) |
| H13  | −0.0316    | 0.7860      | 0.6037        | 0.026*    |
| C14  | 0.1304 (2) | 0.72054 (5) | 0.53793 (14)  | 0.0185 (3) |
| C15  | 0.3081 (3) | 0.79620 (5) | 0.44578 (17)  | 0.0250 (3) |
| H15A | 0.4393     | 0.8062      | 0.3895        | 0.037*    |
| H15B | 0.3181     | 0.8126      | 0.5435        | 0.037*    |
| H15C | 0.1700     | 0.8077      | 0.3929        | 0.037*    |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|-----|------------|------------|------------|------------|-------------|-------------|
| S1  | 0.0248 (2) | 0.01710 (19) | 0.01949 (19) | 0.00449 (11) | 0.00439 (13) | 0.00361 (11) |
| O1  | 0.0270 (5) | 0.0183 (5) | 0.0235 (5) | 0.0047 (4) | 0.0039 (4) | 0.0040 (4) |
| O2  | 0.0211 (5) | 0.0165 (5) | 0.0290 (5) | 0.0017 (4) | 0.0044 (4) | 0.0024 (4) |
| N1  | 0.0179 (5) | 0.0138 (5) | 0.0186 (5) | 0.0023 (4) | 0.0007 (4) | 0.0008 (4) |
| N2  | 0.0173 (5) | 0.0167 (5) | 0.0180 (5) | 0.0011 (4) | 0.0004 (4) | 0.0010 (4) |
| C1  | 0.0177 (6) | 0.0159 (6) | 0.0190 (6) | −0.0019 (5) | −0.0008 (5) | −0.0014 (5) |
| C2  | 0.0175 (6) | 0.0186 (6) | 0.0207 (6) | −0.0025 (5) | −0.0018 (5) | 0.0000 (5) |
| C3  | 0.0170 (6) | 0.0200 (7) | 0.0281 (7) | 0.0000 (5) | −0.0026 (5) | −0.0029 (5) |
| C4  | 0.0199 (6) | 0.0226 (7) | 0.0287 (7) | −0.0019 (5) | 0.0051 (5) | −0.0067 (6) |
| C5  | 0.0288 (7) | 0.0197 (6) | 0.0209 (6) | −0.0029 (5) | 0.0048 (5) | −0.0008 (5) |
| C6  | 0.0245 (7) | 0.0174 (6) | 0.0210 (6) | 0.0001 (5) | 0.0003 (5) | 0.0009 (5) |
| C7  | 0.0180 (6) | 0.0181 (6) | 0.0172 (6) | −0.0001 (5) | −0.0023 (5) | −0.0003 (5) |
| C8  | 0.0158 (6) | 0.0161 (6) | 0.0174 (6) | −0.0004 (5) | −0.0025 (5) | −0.0009 (5) |
| C9  | 0.0170 (6) | 0.0178 (6) | 0.0168 (6) | 0.0031 (5) | −0.0034 (5) | −0.0014 (5) |
| C10 | 0.0179 (6) | 0.0185 (6) | 0.0206 (6) | −0.0002 (5) | −0.0026 (5) | −0.0010 (5) |
| C11 | 0.0177 (6) | 0.0236 (7) | 0.0227 (6) | −0.0003 (5) | −0.0002 (5) | −0.0006 (5) |
| C12 | 0.0193 (6) | 0.0236 (7) | 0.0253 (7) | 0.0047 (5) | 0.0007 (5) | −0.0013 (5) |
| C13 | 0.0223 (7) | 0.0170 (6) | 0.0260 (7) | 0.0034 (5) | −0.0012 (5) | −0.0004 (5) |
| C14 | 0.0172 (6) | 0.0185 (6) | 0.0196 (6) | 0.0006 (5) | −0.0026 (5) | 0.0015 (5) |
| C15 | 0.0279 (7) | 0.0166 (7) | 0.0307 (7) | −0.0013 (5) | 0.0048 (6) | 0.0015 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C8 | 1.6786 (13) | C4—H4 | 0.9500 |
| O1—C7 | 1.2257 (16) | C5—C6 | 1.3862 (19) |
| O2—C14 | 1.3582 (16) | C5—H5 | 0.9500 |
| O2—C15 | 1.4306 (16) | C6—H6 | 0.9500 |
| N1—C7 | 1.3817 (17) | C9—C10 | 1.3865 (18) |
| N1—C8 | 1.3931 (16) | C9—C14 | 1.4147 (18) |
| N1—H1n | 0.902 (18) | C10—C11 | 1.3925 (18) |
| N2—C8 | 1.3322 (17) | C10—H10 | 0.9500 |
| N2—C9 | 1.4140 (16) | C11—C12 | 1.388 (2) |
| N2—H2n | 0.90 (2) | C11—H11 | 0.9500 |
| C1—C6 | 1.3961 (18) | C12—C13 | 1.391 (2) |
| C1—C2 | 1.3969 (18) | C12—H12 | 0.9500 |
| C1—C7 | 1.4893 (18) | C13—C14 | 1.3893 (18) |
| C2—C3 | 1.3921 (18) | C13—H13 | 0.9500 |
| C2—H2 | 0.9500 | C15—H15A | 0.9800 |
| C3—C4 | 1.390 (2) | C15—H15B | 0.9800 |
| C3—H3 | 0.9500 | C15—H15C | 0.9800 |
| C4—C5 | 1.390 (2) | | |
| | | | |
| C14—O2—C15 | 116.92 (10) | N2—C8—N1 | 115.49 (11) |
| C7—N1—C8 | 128.10 (11) | N2—C8—S1 | 126.89 (10) |
| C7—N1—H1n | 116.5 (12) | N1—C8—S1 | 117.61 (9) |
| C8—N1—H1n | 115.2 (12) | C10—C9—N2 | 125.27 (12) |
| C8—N2—C9 | 129.27 (11) | C10—C9—C14 | 119.48 (12) |
| C8—N2—H2n | 114.2 (12) | N2—C9—C14 | 115.12 (11) |
| C9—N2—H2n | 116.4 (12) | C9—C10—C11 | 120.27 (12) |
| C6—C1—C2 | 119.63 (12) | C9—C10—H10 | 119.9 |
| C6—C1—C7 | 117.51 (12) | C11—C10—H10 | 119.9 |
| C2—C1—C7 | 122.80 (12) | C12—C11—C10 | 120.18 (13) |
| C3—C2—C1 | 119.93 (13) | C12—C11—H11 | 119.9 |
| C3—C2—H2 | 120.0 | C10—C11—H11 | 119.9 |
| C1—C2—H2 | 120.0 | C11—C12—C13 | 120.18 (12) |
| C4—C3—C2 | 120.04 (13) | C11—C12—H12 | 119.9 |
| C4—C3—H3 | 120.0 | C13—C12—H12 | 119.9 |
| C2—C3—H3 | 120.0 | C14—C13—C12 | 120.05 (13) |
| C3—C4—C5 | 120.12 (13) | C14—C13—H13 | 120.0 |
| C3—C4—H4 | 119.9 | C12—C13—H13 | 120.0 |
| C5—C4—H4 | 119.9 | O2—C14—C13 | 125.55 (12) |
| C6—C5—C4 | 120.08 (13) | O2—C14—C9 | 114.64 (11) |
| C6—C5—H5 | 120.0 | C13—C14—C9 | 119.80 (12) |
| C4—C5—H5 | 120.0 | O2—C15—H15A | 109.5 |
| C5—C6—C1 | 120.20 (13) | O2—C15—H15B | 109.5 |
| C5—C6—H6 | 119.9 | H15A—C15—H15B | 109.5 |
| C1—C6—H6 | 119.9 | O2—C15—H15C | 109.5 |
| O1—C7—N1 | 122.62 (12) | H15A—C15—H15C | 109.5 |
| O1—C7—C1 | 121.41 (12) | H15B—C15—H15C | 109.5 |

| | | | |
|---|---|---|---|
| N1—C7—C1 | 115.96 (11) | | |
| | | | |
| C6—C1—C2—C3 | −0.12 (19) | C7—N1—C8—S1 | −174.57 (10) |
| C7—C1—C2—C3 | −177.16 (12) | C8—N2—C9—C10 | −33.1 (2) |
| C1—C2—C3—C4 | 0.15 (19) | C8—N2—C9—C14 | 151.20 (13) |
| C2—C3—C4—C5 | −0.3 (2) | N2—C9—C10—C11 | −177.34 (12) |
| C3—C4—C5—C6 | 0.4 (2) | C14—C9—C10—C11 | −1.80 (18) |
| C4—C5—C6—C1 | −0.4 (2) | C9—C10—C11—C12 | −0.1 (2) |
| C2—C1—C6—C5 | 0.2 (2) | C10—C11—C12—C13 | 1.4 (2) |
| C7—C1—C6—C5 | 177.44 (12) | C11—C12—C13—C14 | −0.7 (2) |
| C8—N1—C7—O1 | −2.4 (2) | C15—O2—C14—C13 | −3.32 (19) |
| C8—N1—C7—C1 | 177.36 (12) | C15—O2—C14—C9 | 176.66 (12) |
| C6—C1—C7—O1 | −24.61 (19) | C12—C13—C14—O2 | 178.76 (12) |
| C2—C1—C7—O1 | 152.49 (13) | C12—C13—C14—C9 | −1.23 (19) |
| C6—C1—C7—N1 | 155.68 (12) | C10—C9—C14—O2 | −177.52 (11) |
| C2—C1—C7—N1 | −27.22 (18) | N2—C9—C14—O2 | −1.55 (16) |
| C9—N2—C8—N1 | −179.50 (11) | C10—C9—C14—C13 | 2.46 (19) |
| C9—N2—C8—S1 | −0.8 (2) | N2—C9—C14—C13 | 178.44 (11) |
| C7—N1—C8—N2 | 4.25 (19) | | |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C9–C14 benzene ring.

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| N2—H2n···O1 | 0.905 (18) | 1.867 (18) | 2.6316 (15) | 141.0 (16) |
| C10—H10···S1 | 0.95 | 2.68 | 3.2241 (13) | 117 |
| N2—H2n···O2 | 0.90 (2) | 2.231 (19) | 2.5819 (15) | 102.5 (14) |
| N1—H1n···S1[i] | 0.902 (18) | 2.636 (18) | 3.4976 (12) | 160.1 (15) |
| C15—H15B···O1[ii] | 0.98 | 2.57 | 3.4273 (19) | 146 |
| C15—H15C···Cg1[iii] | 0.98 | 2.81 | 3.6248 (17) | 141 |

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