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# (2*E*)-2-(1,3-Benzothiazol-2-yl)-3-(dimethylamino)prop-2-enenitrile

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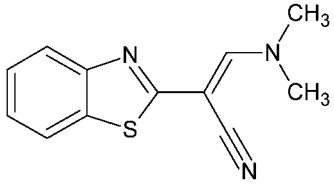
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.037; $wR$ factor = 0.107; data-to-parameter ratio = 14.9.

The molecular conformation of title compound, $C_{12}H_{11}N_3S$, is almost planar [maximum deviation = 0.063 (2) Å]; an intramolecular C—H···N hydrogen bond is noted. In the crystal, molecules interact with each other *via* $\pi$–$\pi$ stacking interactions between thiazole rings [centroid–centroid distance = 3.7475 (9) Å] and methyl-H···$\pi$($C_6$) interactions, forming columns along the *a* axis.

## Related literature

For various biological activities (*e.g.* anti-tumour, anti-inflammatory, anti-viral, *etc.*) of benzothiazole compounds, see: Selvam *et al.* (2011); Sanja & Cvetkovic (2011); Alang *et al.* (2010); Pal *et al.* (2011); Sharma *et al.* (2010); El-Shaaer *et al.* (1997); Gupta & Raat (2010); Hutchinson *et al.* (2002); Gong *et al.* (2004); Hutchinson *et al.* (2003); Geronikaki & Theophilidis (1992); Vicini *et al.* (1990); Das *et al.* (2003); Klose *et al.* (1983); Satsangi *et al.* (1983).




## Experimental

### Crystal data

$C_{12}H_{11}N_3S$
$M_r$ = 229.31
Monoclinic, $P2_1/c$
$a$ = 7.3785 (2) Å
$b$ = 20.1801 (4) Å
$c$ = 8.2706 (2) Å
$\beta$ = 112.947 (4)°
$V$ = 1134.03 (6) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 2.32 mm$^{-1}$
$T$ = 293 K
0.26 × 0.20 × 0.09 mm

### Data collection

Oxford Diffraction SuperNova (Dual, Cu at zero, Atlas) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2013)
$T_{min}$ = 0.584, $T_{max}$ = 0.818
4062 measured reflections
2195 independent reflections
1971 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.016

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.107
$S$ = 1.05
2195 reflections
147 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

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

*Cg*1 is the centroid of the C1–C6 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C9—H9···N1 | 0.93 | 2.44 | 2.851 (2) | 106 |
| C10—H10$A$···$Cg1^{i}$ | 0.96 | 2.77 | 3.549 (2) | 138 |

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2013); 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, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK5279).

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# supplementary materials

*Acta Cryst.* (2014). E**70**, o52–o53 [doi:10.1107/S1600536813033266]

## (2*E*)-2-(1,3-Benzothiazol-2-yl)-3-(dimethylamino)prop-2-enenitrile

**Shaaban K. Mohamed, Mehmet Akkurt, Benson M. Kariuki, Ali M. Ali and Mustafa R. Albayati**

### 1. Comment

It is well known that the thiazolyl group is of great importance in biological systems. In recent years, there has been considerable interest in the synthesis of substituted benzothiazolyl compounds due to their pharmacological properties such as anti-fungal (Selvam *et al.*, 2011; Sanja & Cvetkovic, 2011), anti-viral (Alang *et al.*, 2010; Pal *et al.*, 2011), anti-bacterial (Sharma *et al.*, 2010; El-Shaaer *et al.*, 1997), analgesic (Gupta & Raat, 2010), anti-tumour (Hutchinson *et al.*, 2002) and anti-tuberculosis (Gong *et al.*, 2004; Hutchinson *et al.*, 2003) activities. Moreover, such compounds have been also found to have a potent local anaesthetic activity (Geronikaki & Theophilidis, 1992; Vicini *et al.*, 1990). Anti-inflammatory, analgesic, and anti-pyretic activities for some thiazolyl and benzothiazolyl derivatives are also known (Das *et al*., 2003; Klose *et al.*, 1983; Satsangi *et al.*, 1983). Based on the above and following to our ongoing studies in synthesis of bio-active heterocyclic compounds the title compound has been prepared as a precursor for further study.

As shown in Fig. 1, title compound (I) has an almost planar conformation for non-hydrogen atoms with a maximum deviation of -0.063 (2) Å for C6.

The crystal structure is stabilized by $\pi$-$\pi$ stacking interactions [*Cg*1···*Cg*1(1 - *x*, 1 - *y*, 1 - *z*) = 3.7475 (9) Å; where *Cg*1 is a centroid of the five-membered (S1/N1/C1/C2/C7) thiazole ring of the 1,3-benzothiazole ring system] between the centroids of thiazole rings of the adjacent molecules. The crystal structure has no classical hydrogen bonds. Figs. 2 show the molecular packing of (I) viewed along the a direction.

### 2. Experimental

A mixture of 1,3-benzothiazol-2-ylacetnitrile (174 mg, 1 mmol) and dimethylformamide-dimethylacetal (119 mg, 1 mmol) were taken in acetic acid (10 ml). The reaction mixture was refluxed and monitored by TLC until completion after 8 h. The reaction mixture was allowed to cool at ambient temperature and poured into ice water. The solid product was collected by filtration and recrystallized from ethanol to afford the title compound in 88% yield. Single crystals suitable for X-ray analysis were grown up on slow evaporation of ethanolic solution of the title compound at room temperature over three days. *M*.pt: 441–443 K.

### 3. Refinement

All H-atoms were refined using a riding model with C—H = 0.93 Å and $U_{iso}$=1.2$_{eq}$ (C) for aromatic-H atoms, and C—H = 0.96 Å and $U_{iso}$ = 1.5$U_{eq}$ (C) for methyl-H atoms.

### Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2013); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2013); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2013); 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, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

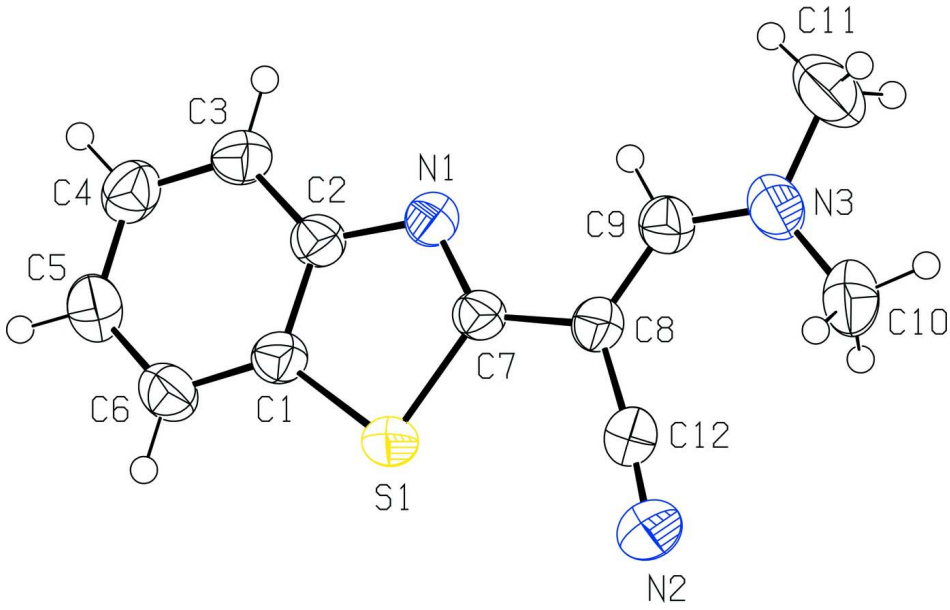


**Figure 1**

The structure of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

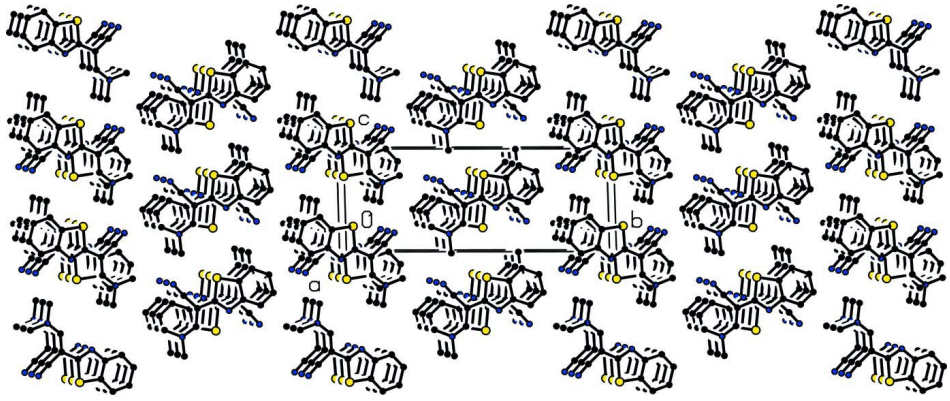


**Figure 2**

The molecular packing of the title compound viewing along the *a* axis. All H atoms are omitted for clarity.

**(2*E*)-2-(1,3-Benzothiazol-2-yl)-3-(dimethylamino)prop-2-enenitrile**

*Crystal data*

$C_{12}H_{11}N_3S$
$M_r = 229.31$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.3785$ (2) Å
$b = 20.1801$ (4) Å
$c = 8.2706$ (2) Å
$\beta = 112.947$ (4)°
$V = 1134.03$ (6) Å$^3$
$Z = 4$
$F(000) = 480$
$D_x = 1.343$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 1971 reflections
$\theta = 4.4$–72.7°
$\mu = 2.32$ mm$^{-1}$
$T = 293$ K
Block, purple
0.26 × 0.20 × 0.09 mm

*Data collection*

Oxford Diffraction SuperNova (Dual, Cu at zero, Atlas) diffractometer
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2013)
$T_{min}$ = 0.584, $T_{max}$ = 0.818
4062 measured reflections
2195 independent reflections
1971 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.016
$\theta_{max}$ = 72.7°, $\theta_{min}$ = 4.4°
$h$ = −7→9
$k$ = −16→25
$l$ = −10→8

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.107
$S$ = 1.05
2195 reflections
147 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0678P)^2 + 0.1211P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.11365 (6) | 0.50492 (2) | 0.23607 (5) | 0.0475 (1) |
| N1 | 0.24456 (18) | 0.46002 (6) | 0.55620 (16) | 0.0427 (4) |
| N2 | 0.3152 (3) | 0.66200 (8) | 0.3024 (2) | 0.0704 (6) |
| N3 | 0.5370 (2) | 0.62896 (8) | 0.81666 (18) | 0.0544 (4) |
| C1 | 0.0527 (2) | 0.42447 (7) | 0.26748 (18) | 0.0417 (4) |
| C2 | 0.1371 (2) | 0.40931 (7) | 0.44773 (19) | 0.0403 (4) |
| C3 | 0.1078 (2) | 0.34624 (8) | 0.5022 (2) | 0.0491 (5) |
| C4 | −0.0040 (3) | 0.30080 (8) | 0.3794 (2) | 0.0518 (5) |
| C5 | −0.0886 (2) | 0.31692 (9) | 0.2020 (2) | 0.0516 (5) |
| C6 | −0.0608 (2) | 0.37875 (9) | 0.1440 (2) | 0.0501 (5) |
| C7 | 0.2450 (2) | 0.51233 (7) | 0.46445 (18) | 0.0388 (4) |
| C8 | 0.3437 (2) | 0.57454 (7) | 0.53589 (19) | 0.0411 (4) |
| C9 | 0.4385 (2) | 0.57944 (8) | 0.7160 (2) | 0.0459 (5) |
| C10 | 0.5596 (3) | 0.69358 (10) | 0.7510 (3) | 0.0643 (6) |
| C11 | 0.6221 (4) | 0.62098 (14) | 1.0073 (3) | 0.0817 (8) |
| C12 | 0.3318 (2) | 0.62455 (8) | 0.4120 (2) | 0.0491 (5) |

| | | | | |
|---|---|---|---|---|
| H3 | 0.16340 | 0.33490 | 0.62050 | 0.0590* |
| H4 | −0.02320 | 0.25870 | 0.41570 | 0.0620* |
| H5 | −0.16480 | 0.28570 | 0.12150 | 0.0620* |
| H6 | −0.11670 | 0.38950 | 0.02530 | 0.0600* |
| H9 | 0.43210 | 0.54140 | 0.77700 | 0.0550* |
| H10A | 0.62640 | 0.68910 | 0.67250 | 0.0960* |
| H10B | 0.63510 | 0.72160 | 0.84750 | 0.0960* |
| H10C | 0.43220 | 0.71290 | 0.68920 | 0.0960* |
| H11A | 0.60670 | 0.57590 | 1.03660 | 0.1230* |
| H11B | 0.55600 | 0.64990 | 1.05890 | 0.1230* |
| H11C | 0.75950 | 0.63200 | 1.05180 | 0.1230* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0628 (3) | 0.0411 (2) | 0.0349 (2) | −0.0012 (2) | 0.0150 (2) | 0.0049 (1) |
| N1 | 0.0501 (7) | 0.0382 (6) | 0.0408 (6) | 0.0023 (5) | 0.0188 (5) | 0.0008 (5) |
| N2 | 0.0975 (13) | 0.0468 (8) | 0.0584 (9) | −0.0053 (8) | 0.0213 (8) | 0.0088 (7) |
| N3 | 0.0544 (7) | 0.0575 (8) | 0.0464 (7) | −0.0001 (6) | 0.0144 (6) | −0.0116 (6) |
| C1 | 0.0489 (7) | 0.0408 (7) | 0.0378 (7) | 0.0023 (6) | 0.0194 (6) | 0.0037 (6) |
| C2 | 0.0457 (7) | 0.0413 (7) | 0.0365 (7) | 0.0036 (6) | 0.0189 (6) | 0.0014 (5) |
| C3 | 0.0618 (9) | 0.0453 (8) | 0.0428 (8) | 0.0007 (7) | 0.0231 (7) | 0.0065 (6) |
| C4 | 0.0642 (9) | 0.0417 (8) | 0.0567 (9) | −0.0033 (7) | 0.0315 (7) | 0.0019 (7) |
| C5 | 0.0575 (9) | 0.0502 (8) | 0.0518 (9) | −0.0093 (7) | 0.0263 (7) | −0.0104 (7) |
| C6 | 0.0576 (9) | 0.0546 (9) | 0.0377 (7) | −0.0041 (7) | 0.0180 (6) | −0.0027 (6) |
| C7 | 0.0443 (7) | 0.0394 (7) | 0.0336 (7) | 0.0066 (5) | 0.0162 (6) | 0.0018 (5) |
| C8 | 0.0457 (7) | 0.0369 (7) | 0.0412 (7) | 0.0041 (6) | 0.0175 (6) | −0.0008 (6) |
| C9 | 0.0486 (8) | 0.0454 (8) | 0.0432 (8) | 0.0039 (6) | 0.0173 (6) | −0.0026 (6) |
| C10 | 0.0652 (10) | 0.0537 (10) | 0.0699 (11) | −0.0082 (8) | 0.0219 (9) | −0.0178 (9) |
| C11 | 0.0848 (15) | 0.0984 (17) | 0.0464 (10) | −0.0053 (13) | 0.0087 (9) | −0.0160 (11) |
| C12 | 0.0570 (9) | 0.0379 (7) | 0.0485 (8) | 0.0002 (6) | 0.0165 (7) | −0.0029 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C1 | 1.7311 (15) | C7—C8 | 1.456 (2) |
| S1—C7 | 1.7612 (14) | C8—C9 | 1.380 (2) |
| N1—C2 | 1.3878 (19) | C8—C12 | 1.416 (2) |
| N1—C7 | 1.3008 (19) | C3—H3 | 0.9300 |
| N2—C12 | 1.150 (2) | C4—H4 | 0.9300 |
| N3—C9 | 1.322 (2) | C5—H5 | 0.9300 |
| N3—C10 | 1.447 (3) | C6—H6 | 0.9300 |
| N3—C11 | 1.461 (3) | C9—H9 | 0.9300 |
| C1—C2 | 1.407 (2) | C10—H10A | 0.9600 |
| C1—C6 | 1.389 (2) | C10—H10B | 0.9600 |
| C2—C3 | 1.395 (2) | C10—H10C | 0.9600 |
| C3—C4 | 1.378 (2) | C11—H11A | 0.9600 |
| C4—C5 | 1.391 (2) | C11—H11B | 0.9600 |
| C5—C6 | 1.381 (3) | C11—H11C | 0.9600 |
| | | | |
| C1—S1—C7 | 89.15 (7) | C2—C3—H3 | 120.00 |

| | | | |
|---|---|---|---|
| C2—N1—C7 | 110.61 (12) | C4—C3—H3 | 120.00 |
| C9—N3—C10 | 124.08 (15) | C3—C4—H4 | 120.00 |
| C9—N3—C11 | 119.72 (17) | C5—C4—H4 | 119.00 |
| C10—N3—C11 | 116.13 (18) | C4—C5—H5 | 120.00 |
| S1—C1—C2 | 109.23 (10) | C6—C5—H5 | 120.00 |
| S1—C1—C6 | 129.06 (12) | C1—C6—H6 | 121.00 |
| C2—C1—C6 | 121.71 (14) | C5—C6—H6 | 121.00 |
| N1—C2—C1 | 115.46 (13) | N3—C9—H9 | 114.00 |
| N1—C2—C3 | 125.84 (13) | C8—C9—H9 | 115.00 |
| C1—C2—C3 | 118.70 (13) | N3—C10—H10A | 109.00 |
| C2—C3—C4 | 119.52 (14) | N3—C10—H10B | 109.00 |
| C3—C4—C5 | 121.02 (16) | N3—C10—H10C | 109.00 |
| C4—C5—C6 | 120.77 (15) | H10A—C10—H10B | 109.00 |
| C1—C6—C5 | 118.27 (14) | H10A—C10—H10C | 109.00 |
| S1—C7—N1 | 115.55 (11) | H10B—C10—H10C | 110.00 |
| S1—C7—C8 | 119.17 (10) | N3—C11—H11A | 109.00 |
| N1—C7—C8 | 125.28 (13) | N3—C11—H11B | 109.00 |
| C7—C8—C9 | 117.55 (13) | N3—C11—H11C | 109.00 |
| C7—C8—C12 | 116.15 (13) | H11A—C11—H11B | 109.00 |
| C9—C8—C12 | 126.30 (14) | H11A—C11—H11C | 110.00 |
| N3—C9—C8 | 131.03 (15) | H11B—C11—H11C | 109.00 |
| N2—C12—C8 | 175.21 (17) | | |

| | | | |
|---|---|---|---|
| C7—S1—C1—C2 | −0.33 (12) | S1—C1—C2—N1 | 0.48 (18) |
| C7—S1—C1—C6 | 179.26 (16) | S1—C1—C2—C3 | −179.33 (12) |
| C1—S1—C7—C8 | −179.85 (13) | N1—C2—C3—C4 | 179.54 (17) |
| C1—S1—C7—N1 | 0.14 (13) | C1—C2—C3—C4 | −0.7 (2) |
| C2—N1—C7—C8 | −179.91 (15) | C2—C3—C4—C5 | −0.2 (3) |
| C7—N1—C2—C3 | 179.41 (16) | C3—C4—C5—C6 | 0.8 (3) |
| C2—N1—C7—S1 | 0.10 (19) | C4—C5—C6—C1 | −0.4 (3) |
| C7—N1—C2—C1 | −0.4 (2) | S1—C7—C8—C12 | −2.3 (2) |
| C11—N3—C9—C8 | 179.2 (2) | N1—C7—C8—C9 | −2.6 (2) |
| C10—N3—C9—C8 | 2.5 (3) | S1—C7—C8—C9 | 177.44 (12) |
| C6—C1—C2—C3 | 1.1 (2) | N1—C7—C8—C12 | 177.71 (15) |
| C6—C1—C2—N1 | −179.15 (15) | C12—C8—C9—N3 | 0.5 (3) |
| S1—C1—C6—C5 | 179.96 (13) | C7—C8—C9—N3 | −179.24 (17) |
| C2—C1—C6—C5 | −0.5 (2) | | |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C1–C6 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C9—H9···N1 | 0.93 | 2.44 | 2.851 (2) | 106 |
| C10—H10*A*···*Cg*1$^{i}$ | 0.96 | 2.77 | 3.549 (2) | 138 |

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.