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# Benzyl *N*′-(1*H*-indol-3-ylmethylidene)-hydrazinecarbodithioate

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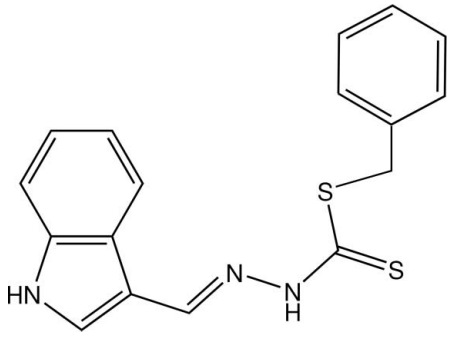
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.049; $wR$ factor = 0.118; data-to-parameter ratio = 17.0.

The $C_{10}H_8N_3S_2$ portion of the title molecule, $C_{17}H_{15}N_3S_3$, is nearly planar (r.m.s. deviation 0.05 Å); this unit and the phenyl ring subtend an angle of 114.5 (2)° at the methylene C atom.

## Related literature

For other Schiff bases derived by condensing *S*-benzyl hydrazinecarbodithioate with either aromatic aldehydes or ketones, see: Ali *et al.* (2004); Chan *et al.* (2003); Fun *et al.* (1995); How *et al.* (2007*a*,*b*,*c*); Khoo *et al.* (2005); Qiu & Luo (2007); Roy *et al.* (2007); Tarafder *et al.* (2002); Xu *et al.* (1991); Zhang *et al.* (2004).




## Experimental

### Crystal data

$C_{17}H_{15}N_3S_2$
$M_r$ = 325.44
Monoclinic, $P2_1/c$
$a$ = 15.4936 (7) Å
$b$ = 9.8114 (4) Å
$c$ = 10.2531 (4) Å
$\beta$ = 98.432 (3)°
$V$ = 1541.8 (1) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.34 mm$^{-1}$
$T$ = 100 (2) K
0.25 × 0.10 × 0.03 mm

### Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.919, $T_{max}$ = 0.990
8531 measured reflections
3383 independent reflections
2323 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.058

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.118
$S$ = 1.01
3383 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.33 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2007); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2309).

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# supplementary materials

*Acta Cryst.* (2008). E**64**, o2107 [ **doi:10.1107/S160053680803198X** ]

# Benzyl *N*'-(1*H*-indol-3-ylmethylidene)hydrazinecarbodithioate

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## Comment

The structure of (I), Fig. 1, shows bond distances for N1—N2 and N2—C9 of 1.382 (3) and 1.287 (3) Å, respectively, confirming the assignment shown in the Scheme. The molecule is bent about the methylene-C7 atom so that the residues on either side are approximately orthogonal. The amino groups do not form any hydrogen bonds.

## Experimental

Indole-3-carbaldehyde (0.37 g, 2.5 mmol) and *S*-benzyl dithiocarbazate (0.50 g, 2.5 mmol) were heated in methanol (40 ml) for 3 h. The solution was set aside for the formation of yellow crystals.

## Refinement

Hydrogen atoms were placed at calculated positions (C—H 0.95–0.99, N—H 0.88 Å) and were treated as riding on their parent carbon atoms, with $U$(H) set to 1.2 times $U_{eq}$(C,N).

## Figures

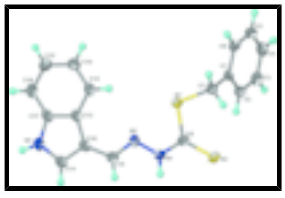


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{17}H_{15}N_2S_3$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

## Benzyl *N*'-(1*H*-indol-3-ylmethylidene)hydrazinecarbodithioate

*Crystal data*

| | |
|---|---|
| $C_{17}H_{15}N_3S_2$ | $F_{000}$ = 680 |
| $M_r$ = 325.44 | $D_x$ = 1.402 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 1305 reflections |
| $a$ = 15.4936 (7) Å | θ = 2.5–23.2° |
| $b$ = 9.8114 (4) Å | μ = 0.34 mm$^{-1}$ |
| $c$ = 10.2531 (4) Å | $T$ = 100 (2) K |
| β = 98.432 (3)° | Prism, light yellow |
| $V$ = 1541.8 (1) Å$^3$ | 0.25 × 0.10 × 0.03 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX diffractometer | 3383 independent reflections |
| Radiation source: fine-focus sealed tube | 2323 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.058$ |
| $T = 100(2)$ K | $\theta_{max} = 27^o$ |
| ω scans | $\theta_{min} = 1.3^o$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h = -20 \rightarrow 20$ |
| $T_{min} = 0.919$, $T_{max} = 0.990$ | $k = -12 \rightarrow 12$ |
| 8531 measured reflections | $l = -13 \rightarrow 8$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.049$ | H-atom parameters constrained |
| $wR(F^2) = 0.118$ | $w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 1.1115P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.01$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 3383 reflections | $\Delta\rho_{max} = 0.48$ e Å$^{-3}$ |
| 199 parameters | $\Delta\rho_{min} = -0.33$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.75015 (5) | 0.74458 (7) | 0.47255 (7) | 0.02090 (18) |
| S2 | 0.87340 (5) | 0.53986 (7) | 0.36891 (7) | 0.02198 (19) |
| N1 | 0.70350 (15) | 0.5227 (2) | 0.3457 (2) | 0.0217 (5) |
| H1 | 0.7086 | 0.4440 | 0.3063 | 0.026* |
| N2 | 0.62145 (15) | 0.5704 (2) | 0.3596 (2) | 0.0212 (5) |
| N3 | 0.32371 (16) | 0.5105 (2) | 0.2983 (2) | 0.0253 (6) |
| H3 | 0.2706 | 0.4795 | 0.2732 | 0.030* |
| C1 | 0.87962 (17) | 0.9360 (3) | 0.4432 (3) | 0.0188 (6) |
| C2 | 0.89308 (18) | 0.9185 (3) | 0.3115 (3) | 0.0216 (6) |
| H2 | 0.8855 | 0.8312 | 0.2714 | 0.026* |
| C3 | 0.91737 (18) | 1.0283 (3) | 0.2403 (3) | 0.0242 (7) |
| H3a | 0.9272 | 1.0156 | 0.1518 | 0.029* |
| C4 | 0.92738 (18) | 1.1564 (3) | 0.2970 (3) | 0.0259 (7) |
| H4 | 0.9436 | 1.2316 | 0.2475 | 0.031* |
| C5 | 0.91353 (19) | 1.1742 (3) | 0.4261 (3) | 0.0245 (7) |
| H5 | 0.9202 | 1.2619 | 0.4654 | 0.029* |
| C6 | 0.89010 (18) | 1.0647 (3) | 0.4983 (3) | 0.0212 (6) |

| | | | | |
|---|---|---|---|---|
| H6 | 0.8811 | 1.0780 | 0.5871 | 0.025* |
| C7 | 0.85739 (18) | 0.8174 (3) | 0.5249 (3) | 0.0210 (6) |
| H7A | 0.8609 | 0.8475 | 0.6176 | 0.025* |
| H7B | 0.9018 | 0.7453 | 0.5220 | 0.025* |
| C8 | 0.77530 (18) | 0.5938 (3) | 0.3909 (3) | 0.0191 (6) |
| C9 | 0.55868 (18) | 0.4859 (3) | 0.3251 (3) | 0.0209 (6) |
| H9 | 0.5717 | 0.3976 | 0.2953 | 0.025* |
| C10 | 0.46972 (19) | 0.5221 (3) | 0.3305 (3) | 0.0204 (6) |
| C11 | 0.39833 (19) | 0.4445 (3) | 0.2826 (3) | 0.0230 (6) |
| H11 | 0.4009 | 0.3569 | 0.2438 | 0.028* |
| C12 | 0.43633 (18) | 0.6451 (3) | 0.3827 (3) | 0.0197 (6) |
| C13 | 0.47407 (19) | 0.7591 (3) | 0.4513 (3) | 0.0217 (6) |
| H13 | 0.5357 | 0.7694 | 0.4680 | 0.026* |
| C14 | 0.42007 (19) | 0.8557 (3) | 0.4939 (3) | 0.0255 (7) |
| H14 | 0.4452 | 0.9328 | 0.5412 | 0.031* |
| C15 | 0.3294 (2) | 0.8434 (3) | 0.4694 (3) | 0.0285 (7) |
| H15 | 0.2941 | 0.9122 | 0.4997 | 0.034* |
| C16 | 0.2901 (2) | 0.7323 (3) | 0.4016 (3) | 0.0284 (7) |
| H16 | 0.2284 | 0.7238 | 0.3842 | 0.034* |
| C17 | 0.34423 (19) | 0.6341 (3) | 0.3602 (3) | 0.0222 (6) |

*Atomic displacement parameters (Å$^2$)*

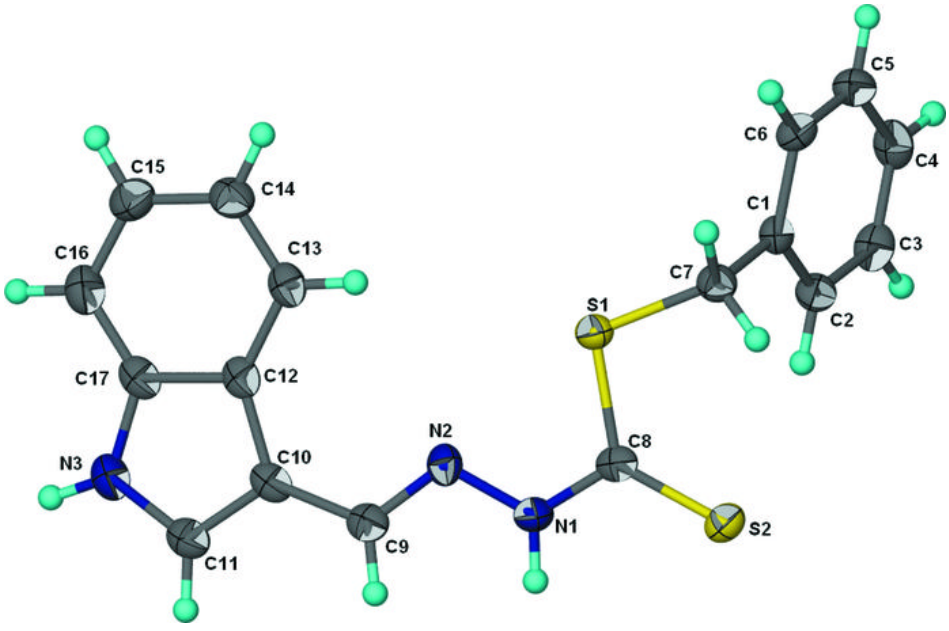
| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0225 (4) | 0.0184 (3) | 0.0229 (4) | −0.0009 (3) | 0.0070 (3) | −0.0025 (3) |
| S2 | 0.0234 (4) | 0.0212 (4) | 0.0226 (4) | 0.0034 (3) | 0.0075 (3) | 0.0014 (3) |
| N1 | 0.0231 (13) | 0.0194 (12) | 0.0234 (14) | −0.0005 (10) | 0.0060 (11) | −0.0047 (10) |
| N2 | 0.0197 (12) | 0.0236 (13) | 0.0211 (14) | −0.0023 (10) | 0.0062 (10) | 0.0016 (11) |
| N3 | 0.0220 (13) | 0.0285 (14) | 0.0249 (14) | −0.0048 (11) | 0.0022 (11) | 0.0006 (11) |
| C1 | 0.0166 (14) | 0.0203 (14) | 0.0195 (16) | −0.0007 (11) | 0.0027 (12) | 0.0006 (12) |
| C2 | 0.0223 (15) | 0.0239 (15) | 0.0181 (16) | −0.0013 (12) | 0.0012 (12) | −0.0037 (12) |
| C3 | 0.0235 (15) | 0.0337 (17) | 0.0158 (15) | 0.0008 (13) | 0.0038 (12) | 0.0034 (13) |
| C4 | 0.0236 (15) | 0.0250 (15) | 0.0295 (19) | −0.0006 (13) | 0.0045 (13) | 0.0106 (14) |
| C5 | 0.0262 (16) | 0.0198 (15) | 0.0277 (18) | 0.0005 (12) | 0.0041 (13) | −0.0016 (13) |
| C6 | 0.0228 (15) | 0.0218 (15) | 0.0196 (16) | 0.0036 (12) | 0.0050 (12) | −0.0002 (12) |
| C7 | 0.0227 (15) | 0.0209 (15) | 0.0196 (16) | −0.0006 (12) | 0.0032 (12) | −0.0010 (12) |
| C8 | 0.0265 (15) | 0.0170 (14) | 0.0149 (15) | 0.0008 (11) | 0.0064 (12) | 0.0024 (11) |
| C9 | 0.0277 (16) | 0.0217 (15) | 0.0142 (15) | −0.0022 (12) | 0.0058 (12) | −0.0003 (12) |
| C10 | 0.0268 (15) | 0.0201 (14) | 0.0140 (15) | −0.0048 (12) | 0.0020 (12) | 0.0024 (12) |
| C11 | 0.0297 (16) | 0.0217 (15) | 0.0180 (16) | −0.0046 (13) | 0.0054 (13) | 0.0009 (13) |
| C12 | 0.0233 (15) | 0.0220 (15) | 0.0143 (15) | −0.0039 (12) | 0.0044 (12) | 0.0040 (12) |
| C13 | 0.0227 (15) | 0.0248 (15) | 0.0177 (16) | −0.0043 (12) | 0.0037 (12) | 0.0041 (13) |
| C14 | 0.0315 (17) | 0.0253 (16) | 0.0205 (17) | −0.0039 (13) | 0.0063 (13) | −0.0028 (13) |
| C15 | 0.0291 (17) | 0.0296 (17) | 0.0277 (18) | 0.0022 (14) | 0.0077 (14) | −0.0038 (14) |
| C16 | 0.0231 (16) | 0.0340 (18) | 0.0281 (18) | −0.0034 (13) | 0.0040 (13) | 0.0005 (15) |
| C17 | 0.0272 (16) | 0.0228 (15) | 0.0163 (15) | −0.0057 (12) | 0.0025 (12) | 0.0034 (12) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—C8 | 1.771 (3) | C5—H5 | 0.9500 |
| S1—C7 | 1.816 (3) | C6—H6 | 0.9500 |
| S2—C8 | 1.656 (3) | C7—H7A | 0.9900 |
| N1—C8 | 1.337 (4) | C7—H7B | 0.9900 |
| N1—N2 | 1.382 (3) | C9—C10 | 1.432 (4) |
| N1—H1 | 0.8800 | C9—H9 | 0.9500 |
| N2—C9 | 1.287 (3) | C10—C11 | 1.373 (4) |
| N3—C11 | 1.355 (4) | C10—C12 | 1.446 (4) |
| N3—C17 | 1.384 (4) | C11—H11 | 0.9500 |
| N3—H3 | 0.8800 | C12—C13 | 1.402 (4) |
| C1—C6 | 1.383 (4) | C12—C17 | 1.416 (4) |
| C1—C2 | 1.407 (4) | C13—C14 | 1.377 (4) |
| C1—C7 | 1.503 (4) | C13—H13 | 0.9500 |
| C2—C3 | 1.384 (4) | C14—C15 | 1.395 (4) |
| C2—H2 | 0.9500 | C14—H14 | 0.9500 |
| C3—C4 | 1.384 (4) | C15—C16 | 1.385 (4) |
| C3—H3a | 0.9500 | C15—H15 | 0.9500 |
| C4—C5 | 1.384 (4) | C16—C17 | 1.384 (4) |
| C4—H4 | 0.9500 | C16—H16 | 0.9500 |
| C5—C6 | 1.383 (4) | | |
| C8—S1—C7 | 102.30 (13) | H7A—C7—H7B | 107.6 |
| C8—N1—N2 | 121.2 (2) | N1—C8—S2 | 121.3 (2) |
| C8—N1—H1 | 119.4 | N1—C8—S1 | 111.7 (2) |
| N2—N1—H1 | 119.4 | S2—C8—S1 | 126.97 (17) |
| C9—N2—N1 | 115.0 (2) | N2—C9—C10 | 121.5 (3) |
| C11—N3—C17 | 109.3 (2) | N2—C9—H9 | 119.3 |
| C11—N3—H3 | 125.4 | C10—C9—H9 | 119.3 |
| C17—N3—H3 | 125.4 | C11—C10—C9 | 125.3 (3) |
| C6—C1—C2 | 118.6 (3) | C11—C10—C12 | 106.4 (3) |
| C6—C1—C7 | 120.1 (3) | C9—C10—C12 | 128.3 (3) |
| C2—C1—C7 | 121.2 (3) | N3—C11—C10 | 110.4 (3) |
| C3—C2—C1 | 120.1 (3) | N3—C11—H11 | 124.8 |
| C3—C2—H2 | 119.9 | C10—C11—H11 | 124.8 |
| C1—C2—H2 | 119.9 | C13—C12—C17 | 118.6 (3) |
| C4—C3—C2 | 120.5 (3) | C13—C12—C10 | 134.9 (3) |
| C4—C3—H3a | 119.8 | C17—C12—C10 | 106.4 (2) |
| C2—C3—H3a | 119.8 | C14—C13—C12 | 118.7 (3) |
| C3—C4—C5 | 119.5 (3) | C14—C13—H13 | 120.7 |
| C3—C4—H4 | 120.2 | C12—C13—H13 | 120.7 |
| C5—C4—H4 | 120.2 | C13—C14—C15 | 121.7 (3) |
| C4—C5—C6 | 120.3 (3) | C13—C14—H14 | 119.2 |
| C4—C5—H5 | 119.9 | C15—C14—H14 | 119.2 |
| C6—C5—H5 | 119.9 | C16—C15—C14 | 121.0 (3) |
| C5—C6—C1 | 121.0 (3) | C16—C15—H15 | 119.5 |
| C5—C6—H6 | 119.5 | C14—C15—H15 | 119.5 |
| C1—C6—H6 | 119.5 | C17—C16—C15 | 117.4 (3) |

| | | | |
|---|---|---|---|
| C1—C7—S1 | 114.5 (2) | C17—C16—H16 | 121.3 |
| C1—C7—H7A | 108.6 | C15—C16—H16 | 121.3 |
| S1—C7—H7A | 108.6 | C16—C17—N3 | 129.9 (3) |
| C1—C7—H7B | 108.6 | C16—C17—C12 | 122.6 (3) |
| S1—C7—H7B | 108.6 | N3—C17—C12 | 107.4 (2) |
| C8—N1—N2—C9 | −172.7 (3) | C9—C10—C11—N3 | −177.4 (3) |
| C6—C1—C2—C3 | 0.8 (4) | C12—C10—C11—N3 | 1.3 (3) |
| C7—C1—C2—C3 | −177.1 (3) | C11—C10—C12—C13 | 175.2 (3) |
| C1—C2—C3—C4 | −1.0 (4) | C9—C10—C12—C13 | −6.2 (5) |
| C2—C3—C4—C5 | 0.5 (4) | C11—C10—C12—C17 | −1.0 (3) |
| C3—C4—C5—C6 | 0.2 (4) | C9—C10—C12—C17 | 177.7 (3) |
| C4—C5—C6—C1 | −0.3 (4) | C17—C12—C13—C14 | 0.0 (4) |
| C2—C1—C6—C5 | −0.2 (4) | C10—C12—C13—C14 | −175.8 (3) |
| C7—C1—C6—C5 | 177.7 (3) | C12—C13—C14—C15 | −0.6 (4) |
| C6—C1—C7—S1 | 113.9 (3) | C13—C14—C15—C16 | 0.4 (5) |
| C2—C1—C7—S1 | −68.2 (3) | C14—C15—C16—C17 | 0.4 (5) |
| C8—S1—C7—C1 | 103.7 (2) | C15—C16—C17—N3 | 175.7 (3) |
| N2—N1—C8—S2 | −177.5 (2) | C15—C16—C17—C12 | −1.1 (4) |
| N2—N1—C8—S1 | 2.6 (3) | C11—N3—C17—C16 | −176.7 (3) |
| C7—S1—C8—N1 | 179.0 (2) | C11—N3—C17—C12 | 0.4 (3) |
| C7—S1—C8—S2 | −0.9 (2) | C13—C12—C17—C16 | 0.9 (4) |
| N1—N2—C9—C10 | −178.3 (2) | C10—C12—C17—C16 | 177.8 (3) |
| N2—C9—C10—C11 | 172.6 (3) | C13—C12—C17—N3 | −176.6 (2) |
| N2—C9—C10—C12 | −5.8 (5) | C10—C12—C17—N3 | 0.3 (3) |
| C17—N3—C11—C10 | −1.1 (3) | | |

**Fig. 1**


C5
C6
C4
C1
C3
C7
S1
C2
C15
C14
C16
C13
C17
C12
N2
C8
N3
C10
N1
S2
C9
C11