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2-(1,3-Benzothiazol-2-yliminomethyl)-2-naphthol

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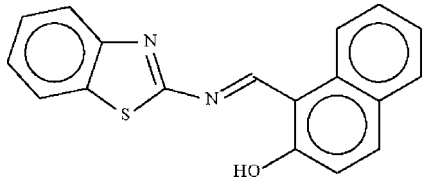
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.122; data-to-parameter ratio = 15.5.

In the title molecule, $C_{18}H_{12}N_2OS$, the dihedral angle between the two fused-ring systems is 7.2 (1)°. The hydroxy group forms an intramolecular hydrogen bond with the imino group.

Related literature

For the crystal structures of other Schiff bases derived by condensing benzthiazolyl-2-amine with aldehydes/ketones, see: Büyükgüngör *et al.* (2004); Cannon *et al.* (2001); Guo *et al.* (2002); Saraçoğlu *et al.* (2004).



Experimental

Crystal data

$C_{18}H_{12}N_2OS$
M_r = 304.36
Monoclinic, $P2_1/n$
a = 9.6398 (2) Å
b = 14.9687 (4) Å
c = 9.6646 (2) Å
β = 101.323 (2)°
V = 1367.41 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 123 K
0.25 × 0.20 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.943, T_{max} = 0.988
12442 measured reflections
3139 independent reflections
2396 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.122
S = 1.02
3139 reflections
203 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.84 (1)	1.82 (2)	2.573 (2)	148 (3)

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; 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, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2783).

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supplementary materials

Acta Cryst. (2009). E**65**, o759 [**doi:10.1107/S1600536809008514**]

2-(1,3-Benzothiazol-2-yliminomethyl)-2-naphthol

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Comment

The molecular structure of the title compound is shown in Fig. 1.

Experimental

2-Aminobenzothiazole (4.0 g, 26.6 mmol) dissolved in ethanol (25 ml) was added to 2-hydroxybenzaldehyde (4.58 g, 26.6 mmol) dissolved in ethanol (25 ml). The mixture was heated for another hour. The solid that separated from the reaction mixture was isolated and recrystallized from ethanol.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.95 Å) and were included in the refinement in the riding model approximation, with *U*(H) fixed at 1.2*U*(C).

The hydroxy H-atom was located in a difference Fouier map, and was refined with a distance restraint of O–H 0.84±0.01 Å; its isotropic displacement parameter was refined.

Figures

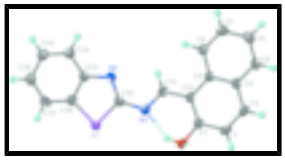


Fig. 1. Thermal ellisoid plot (Barbour, 2001) of $C_{18}H_{12}N_2OS$; probability levels are set at 70% and H-atoms are drawn as spheres of arbitrary radius. The dashed line denotes the hydrogen bond.

2-(1,3-Benzothiazol-2-yliminomethyl)-2-naphthol

Crystal data

$C_{18}H_{12}N_2OS$	F_{000} = 632
M_r = 304.36	D_x = 1.481 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2677 reflections
a = 9.6398 (2) Å	θ = 2.5–28.1°
b = 14.9687 (4) Å	μ = 0.24 mm^{-1}
c = 9.6646 (2) Å	T = 123 K
β = 101.323 (2)°	Irregular block, orange
V = 1367.41 (5) Å^3	0.25 × 0.20 × 0.05 mm

$Z = 4$

Data collection

Bruker SMART APEX diffractometer	3139 independent reflections
Radiation source: fine-focus sealed tube	2396 reflections with $I > 2\tilde{}I$)
Monochromator: graphite	$R_{int} = 0.051$
$T = 123$ K	$\theta_{max} = 27.5^{o}$
ω scans	$\theta_{min} = 2.5^{o}$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{min} = 0.943$, $T_{max} = 0.988$	$k = -19 \rightarrow 19$
12442 measured reflections	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.122$	$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2 + 0.543P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
3139 reflections	$\Delta\rho_{max} = 0.53$ e Å^{-3}
203 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.62414 (5)	0.57067 (3)	0.89471 (5)	0.02326 (15)
O1	0.28598 (15)	0.35583 (9)	0.77536 (15)	0.0261 (3)
H1	0.348 (2)	0.3964 (14)	0.782 (3)	0.057 (9)*
N1	0.41330 (16)	0.49518 (10)	0.70645 (17)	0.0214 (4)
N2	0.53279 (16)	0.62326 (11)	0.63631 (17)	0.0218 (3)
C1	0.19789 (19)	0.36352 (12)	0.6498 (2)	0.0207 (4)
C2	0.0903 (2)	0.29840 (13)	0.6173 (2)	0.0236 (4)

H2	0.0831	0.2524	0.6833	0.028*
C3	−0.0028 (2)	0.30118 (13)	0.4924 (2)	0.0227 (4)
H3	−0.0733	0.2562	0.4715	0.027*
C4	0.00270 (19)	0.37013 (12)	0.3918 (2)	0.0205 (4)
C5	−0.0966 (2)	0.37268 (13)	0.2635 (2)	0.0242 (4)
H5	−0.1667	0.3274	0.2434	0.029*
C6	−0.0935 (2)	0.43936 (14)	0.1678 (2)	0.0257 (4)
H6	−0.1613	0.4407	0.0819	0.031*
C7	0.0109 (2)	0.50600 (13)	0.1975 (2)	0.0246 (4)
H7	0.0131	0.5526	0.1312	0.030*
C8	0.1093 (2)	0.50481 (13)	0.3206 (2)	0.0219 (4)
H8	0.1790	0.5504	0.3380	0.026*
C9	0.10912 (19)	0.43680 (12)	0.42252 (19)	0.0189 (4)
C10	0.20982 (19)	0.43225 (12)	0.5546 (2)	0.0190 (4)
C11	0.3197 (2)	0.49736 (13)	0.5896 (2)	0.0210 (4)
H11	0.3245	0.5443	0.5245	0.025*
C12	0.51359 (19)	0.56351 (12)	0.7280 (2)	0.0205 (4)
C13	0.64047 (19)	0.68133 (12)	0.6951 (2)	0.0199 (4)
C14	0.6849 (2)	0.75430 (13)	0.6250 (2)	0.0230 (4)
H14	0.6414	0.7675	0.5303	0.028*
C15	0.7934 (2)	0.80674 (13)	0.6964 (2)	0.0251 (4)
H15	0.8252	0.8562	0.6495	0.030*
C16	0.8576 (2)	0.78866 (13)	0.8360 (2)	0.0256 (4)
H16	0.9320	0.8260	0.8826	0.031*
C17	0.8139 (2)	0.71684 (13)	0.9077 (2)	0.0245 (4)
H17	0.8570	0.7046	1.0029	0.029*
C18	0.7052 (2)	0.66319 (13)	0.8359 (2)	0.0214 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0230 (3)	0.0244 (3)	0.0214 (3)	−0.00141 (19)	0.00199 (18)	0.00103 (19)
O1	0.0272 (7)	0.0245 (8)	0.0252 (7)	−0.0027 (6)	0.0017 (6)	0.0047 (6)
N1	0.0198 (8)	0.0208 (8)	0.0237 (8)	−0.0009 (6)	0.0049 (6)	−0.0016 (7)
N2	0.0210 (8)	0.0221 (8)	0.0220 (8)	−0.0008 (6)	0.0034 (6)	−0.0001 (7)
C1	0.0204 (9)	0.0202 (9)	0.0224 (10)	0.0019 (7)	0.0065 (7)	−0.0006 (7)
C2	0.0261 (10)	0.0194 (9)	0.0276 (10)	−0.0001 (8)	0.0112 (8)	0.0027 (8)
C3	0.0211 (9)	0.0188 (9)	0.0301 (11)	−0.0030 (7)	0.0098 (8)	−0.0036 (8)
C4	0.0197 (9)	0.0193 (9)	0.0241 (10)	0.0010 (7)	0.0081 (7)	−0.0031 (8)
C5	0.0198 (9)	0.0231 (10)	0.0295 (11)	−0.0015 (8)	0.0045 (8)	−0.0066 (8)
C6	0.0240 (10)	0.0278 (11)	0.0235 (10)	0.0055 (8)	0.0006 (8)	−0.0047 (8)
C7	0.0280 (10)	0.0238 (10)	0.0230 (10)	0.0048 (8)	0.0074 (8)	0.0007 (8)
C8	0.0227 (9)	0.0194 (9)	0.0249 (10)	−0.0009 (7)	0.0078 (8)	−0.0013 (8)
C9	0.0185 (9)	0.0178 (9)	0.0216 (9)	0.0025 (7)	0.0067 (7)	−0.0019 (7)
C10	0.0183 (9)	0.0176 (9)	0.0223 (9)	0.0018 (7)	0.0072 (7)	−0.0015 (7)
C11	0.0218 (9)	0.0192 (9)	0.0236 (10)	0.0007 (7)	0.0082 (7)	0.0005 (8)
C12	0.0191 (9)	0.0213 (9)	0.0210 (9)	0.0024 (7)	0.0035 (7)	−0.0024 (7)
C13	0.0181 (9)	0.0186 (9)	0.0236 (10)	0.0031 (7)	0.0053 (7)	−0.0030 (7)

C14	0.0229 (9)	0.0213 (10)	0.0247 (10)	0.0020 (8)	0.0050 (8)	−0.0003 (8)
C15	0.0256 (10)	0.0201 (10)	0.0311 (11)	0.0003 (8)	0.0093 (8)	−0.0006 (8)
C16	0.0214 (9)	0.0235 (10)	0.0319 (11)	−0.0011 (8)	0.0057 (8)	−0.0065 (8)
C17	0.0223 (10)	0.0280 (11)	0.0229 (10)	0.0028 (8)	0.0037 (8)	−0.0041 (8)
C18	0.0204 (9)	0.0220 (9)	0.0227 (10)	0.0028 (8)	0.0067 (7)	−0.0026 (8)

Geometric parameters (Å, °)

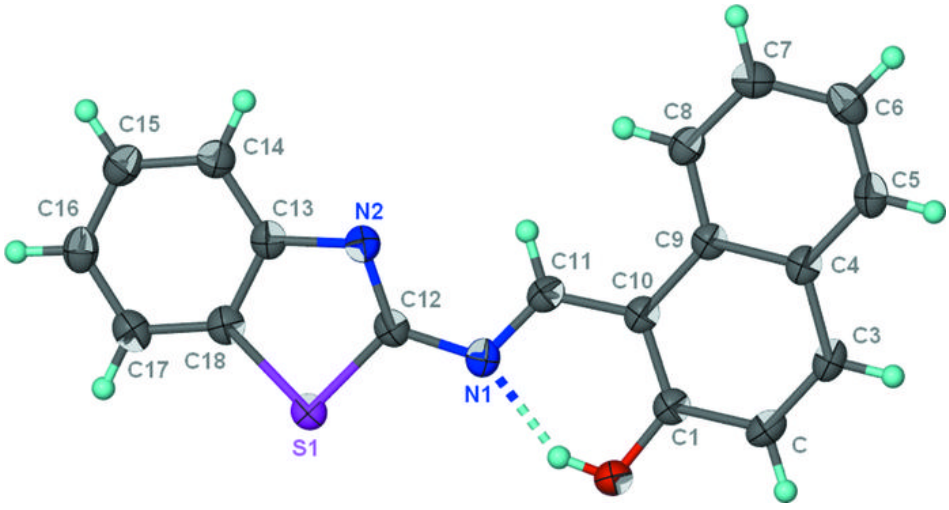
S1—C18	1.740 (2)	C6—H6	0.9500
S1—C12	1.7519 (19)	C7—C8	1.368 (3)
O1—C1	1.343 (2)	C7—H7	0.9500
O1—H1	0.843 (10)	C8—C9	1.417 (3)
N1—C11	1.300 (2)	C8—H8	0.9500
N1—C12	1.395 (2)	C9—C10	1.445 (3)
N2—C12	1.298 (2)	C10—C11	1.430 (3)
N2—C13	1.387 (2)	C11—H11	0.9500
C1—C10	1.400 (3)	C13—C14	1.396 (3)
C1—C2	1.413 (3)	C13—C18	1.408 (3)
C2—C3	1.356 (3)	C14—C15	1.380 (3)
C2—H2	0.9500	C14—H14	0.9500
C3—C4	1.426 (3)	C15—C16	1.397 (3)
C3—H3	0.9500	C15—H15	0.9500
C4—C5	1.410 (3)	C16—C17	1.388 (3)
C4—C9	1.420 (3)	C16—H16	0.9500
C5—C6	1.365 (3)	C17—C18	1.392 (3)
C5—H5	0.9500	C17—H17	0.9500
C6—C7	1.406 (3)		
C18—S1—C12	88.83 (9)	C8—C9—C10	123.76 (17)
C1—O1—H1	109 (2)	C4—C9—C10	118.92 (17)
C11—N1—C12	116.99 (16)	C1—C10—C11	119.86 (17)
C12—N2—C13	110.36 (16)	C1—C10—C9	119.17 (17)
O1—C1—C10	122.56 (17)	C11—C10—C9	120.96 (17)
O1—C1—C2	116.63 (17)	N1—C11—C10	122.94 (18)
C10—C1—C2	120.82 (18)	N1—C11—H11	118.5
C3—C2—C1	120.34 (18)	C10—C11—H11	118.5
C3—C2—H2	119.8	N2—C12—N1	126.25 (17)
C1—C2—H2	119.8	N2—C12—S1	116.32 (14)
C2—C3—C4	121.51 (18)	N1—C12—S1	117.44 (14)
C2—C3—H3	119.2	N2—C13—C14	124.58 (17)
C4—C3—H3	119.2	N2—C13—C18	115.42 (17)
C5—C4—C9	120.17 (18)	C14—C13—C18	120.00 (17)
C5—C4—C3	120.62 (17)	C15—C14—C13	118.50 (18)
C9—C4—C3	119.21 (18)	C15—C14—H14	120.8
C6—C5—C4	120.93 (18)	C13—C14—H14	120.7
C6—C5—H5	119.5	C14—C15—C16	121.43 (19)
C4—C5—H5	119.5	C14—C15—H15	119.3
C5—C6—C7	119.37 (19)	C16—C15—H15	119.3
C5—C6—H6	120.3	C17—C16—C15	120.81 (19)
C7—C6—H6	120.3	C17—C16—H16	119.6

C8—C7—C6	120.97 (19)	C15—C16—H16	119.6
C8—C7—H7	119.5	C16—C17—C18	118.07 (19)
C6—C7—H7	119.5	C16—C17—H17	121.0
C7—C8—C9	121.24 (18)	C18—C17—H17	121.0
C7—C8—H8	119.4	C17—C18—C13	121.18 (18)
C9—C8—H8	119.4	C17—C18—S1	129.72 (16)
C8—C9—C4	117.32 (17)	C13—C18—S1	109.07 (14)
O1—C1—C2—C3	−179.77 (17)	C12—N1—C11—C10	−179.24 (16)
C10—C1—C2—C3	0.5 (3)	C1—C10—C11—N1	1.6 (3)
C1—C2—C3—C4	−1.3 (3)	C9—C10—C11—N1	−179.23 (17)
C2—C3—C4—C5	−178.90 (18)	C13—N2—C12—N1	179.17 (17)
C2—C3—C4—C9	0.7 (3)	C13—N2—C12—S1	−0.3 (2)
C9—C4—C5—C6	−0.8 (3)	C11—N1—C12—N2	−8.4 (3)
C3—C4—C5—C6	178.85 (18)	C11—N1—C12—S1	171.09 (14)
C4—C5—C6—C7	0.4 (3)	C18—S1—C12—N2	−0.17 (15)
C5—C6—C7—C8	0.2 (3)	C18—S1—C12—N1	−179.72 (15)
C6—C7—C8—C9	−0.3 (3)	C12—N2—C13—C14	−178.50 (17)
C7—C8—C9—C4	−0.1 (3)	C12—N2—C13—C18	0.8 (2)
C7—C8—C9—C10	−179.70 (17)	N2—C13—C14—C15	179.92 (17)
C5—C4—C9—C8	0.6 (3)	C18—C13—C14—C15	0.6 (3)
C3—C4—C9—C8	−179.03 (16)	C13—C14—C15—C16	−0.6 (3)
C5—C4—C9—C10	−179.76 (16)	C14—C15—C16—C17	0.1 (3)
C3—C4—C9—C10	0.6 (3)	C15—C16—C17—C18	0.4 (3)
O1—C1—C10—C11	0.4 (3)	C16—C17—C18—C13	−0.4 (3)
C2—C1—C10—C11	−179.91 (17)	C16—C17—C18—S1	−178.59 (15)
O1—C1—C10—C9	−178.88 (16)	N2—C13—C18—C17	−179.46 (17)
C2—C1—C10—C9	0.9 (3)	C14—C13—C18—C17	−0.1 (3)
C8—C9—C10—C1	178.24 (17)	N2—C13—C18—S1	−0.9 (2)
C4—C9—C10—C1	−1.4 (3)	C14—C13—C18—S1	178.42 (14)
C8—C9—C10—C11	−1.0 (3)	C12—S1—C18—C17	178.94 (19)
C4—C9—C10—C11	179.39 (17)	C12—S1—C18—C13	0.60 (14)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.84 (1)	1.82 (2)	2.573 (2)	148 (3)

Fig. 1


C7
C8
C6
C5
C15
C14
C16
C13
N2
C9
C4
C11
C10
C12
C3
C17
C18
N1
S1
C1
C