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1-[(*S*)-1-Phenylethyl]-1*H*-benzimidazole

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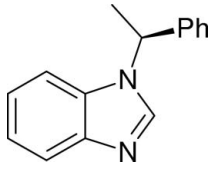
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.080; data-to-parameter ratio = 10.1.

In the chiral title compound, $C_{15}H_{14}N_2$, the dihedral angle between the mean planes of the aromatic rings is 81.59 (4)°. An intermolecular C—H···N interaction (H···N = 2.50 Å) involving the chiral C atom results in [100] chains of molecules in the crystal structure.

Related literature

The synthesis of the title compound was recently reported by Rivas *et al.* (2002).

For bond-length data, see: Allen *et al.* (1987). For graph-set notation, see: Etter (1990).



Experimental

Crystal data

$C_{15}H_{14}N_2$
M_r = 222.28
Orthorhombic, $P2_12_12_1$
a = 6.3159 (3) Å
b = 8.6989 (3) Å
c = 21.3277 (9) Å
V = 1171.77 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 120 (2) K
0.46 × 0.20 × 0.13 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.966, T_{max} = 0.990
8654 measured reflections
1571 independent reflections
1463 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.081
S = 1.05
1571 reflections
156 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···N2^{i}	1.00	2.50	3.422 (2)	152

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997), and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

We thank the EPSRC National Crystallography Service (University of Southampton) for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2136).

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supplementary materials

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1-[(*S*)-1-Phenylethyl]-1*H*-benzimidazole

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Comment

The title compound (Fig. 1) was prepared as a possible component of a chiral catalyst. The same compound was recently reported by Rivas *et al.* (2002).

The geometrical parameters may be regarded as normal (Allen *et al.*, 1987). The dihedral angle between the mean planes of the C1—C7/N1/N2 fused ring and C10—C15 ring is 81.59 (4)°. Atom C8 of the title molecule is chiral: S configuration was assigned to this atom based on the known chirality of the equivalent atom in the starting material.

The crystal packing is consolidated by a C8—H8···N2^{i} interaction (Table 1), which links the molecules into [100] chains (Fig. 2) with a C(5) graph-set motif (Etter, 1990). There are no π-π stacking interactions, as the minimum separation of the centroids of the aromatic rings of nearby molecules is greater than 5 Å.

Experimental

N-((*S*)-1-Phenyl-ethyl)-benzene-1,2-diamine (8.479 g, 39.9 mmol) was placed in a flask, and dissolved in $HC(OEt)_3$ (85 ml). *p*-Toluenesulphonic acid (0.340 g, 1.7 mmol, 5 mol%) was added, and the solution heated at 353 K for 24 h. Removal of volatiles *in vacuo* gave a yellow oil, which was partitioned between aqueous Na_2CO_3 solution (5% *w*/*v*, 200 ml) and DCM (3 τimes 200 ml). The combined organics were dried ($MgSO_4$), and solvent removed to yield pale yellow plates (3.323 g, 37%). Slow evaporation of a DCM solution produced colourless crystals of (I) suitable for diffraction; mp 418–420 K; $[\alpha]_D$ −9.3 (c = 1.73, DCM); $C_{15}H_{14}N_2$ requires C 81.05, H 6.35, N 12.60%; found C 81.21, H 6.38, N 12.64%.

Refinement

Anomalous dispersion was negligible and Friedel pairs were merged before refinement. The S chirality at C8 was assigned based on the known chirality of the equivalent atom in the starting material. The hydrogen atoms were placed in calculated positions (C—H = 0.95–1.00 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The –CH_3 group was allowed to rotate but not to tip, to best fit the electron density.

Figures

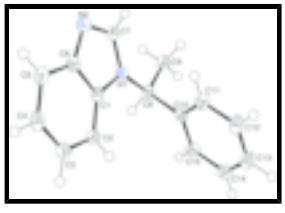

Fig. 1. View of the molecular structure showing 50% displacement ellipsoids (H atoms are drawn as small spheres of arbitrary radius).

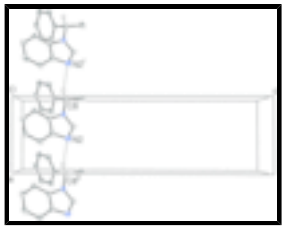

Fig. 2. Fragement of the crystal structure showing part of a [100] chain of molecules linked by C—H···N bonds (double dashed lines). All H atoms except H8 are omitted for clarity. Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$.

1-[(*S*)-1-Phenylethyl]-1*H*-benzimidazole

Crystal data

$C_{15}H_{14}N_2$	$F_{000} = 472$
$M_r = 222.28$	$D_x = 1.260$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 1583 reflections
$a = 6.3159$ (3) Å	$\theta = 2.9$–27.5º
$b = 8.6989$ (3) Å	$\mu = 0.08$ mm^{-1}
$c = 21.3277$ (9) Å	$T = 120$ (2) K
$V = 1171.77$ (8) Å^3	Shard, colourless
$Z = 4$	0.46 × 0.20 × 0.13 mm

Data collection

Nonius KappaCCD diffractometer	1571 independent reflections
Radiation source: fine-focus sealed tube	1463 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.039$
$T = 120(2)$ K	$\theta_{max} = 27.5$º
ω and φ scans	$\theta_{min} = 3.0$º
Absorption correction: multi-scan (SADABS; Bruker, 2003)	$h = -8\rightarrow8$
$T_{min} = 0.966$, $T_{max} = 0.990$	$k = -9\rightarrow11$
8654 measured reflections	$l = -27\rightarrow27$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.032$	$w = 1/[\sigma^2(F_o^2) + (0.0349P)^2 + 0.2819P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.081$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.05$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
1571 reflections	$\Delta\rho_{min} = -0.17$ e Å^{-3}
156 parameters	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Extinction coefficient: 0.033 (6)

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.2835 (3)	0.24132 (17)	0.13869 (7)	0.0194 (3)
C2	0.1813 (3)	0.21889 (19)	0.08162 (7)	0.0235 (4)
H2	0.0451	0.2607	0.0735	0.028*
C3	0.2884 (3)	0.13264 (19)	0.03749 (8)	0.0264 (4)
H3	0.2243	0.1150	−0.0022	0.032*
C4	0.4891 (3)	0.0703 (2)	0.04954 (8)	0.0270 (4)
H4	0.5580	0.0121	0.0179	0.032*
C5	0.5886 (3)	0.09180 (19)	0.10661 (8)	0.0251 (4)
H5	0.7241	0.0488	0.1148	0.030*
C6	0.4826 (3)	0.17917 (19)	0.15197 (7)	0.0213 (3)
C7	0.3886 (3)	0.3043 (2)	0.23324 (8)	0.0229 (4)
H7	0.3884	0.3491	0.2739	0.027*
C8	0.0229 (3)	0.40316 (18)	0.19948 (7)	0.0198 (3)
H8	−0.0933	0.3274	0.1918	0.024*
C9	−0.0023 (3)	0.4646 (2)	0.26587 (7)	0.0262 (4)
H9A	0.0136	0.3800	0.2959	0.039*
H9B	−0.1430	0.5107	0.2706	0.039*
H9C	0.1063	0.5426	0.2739	0.039*
C10	0.0007 (3)	0.53183 (18)	0.15155 (7)	0.0196 (3)
C11	0.1706 (3)	0.62418 (19)	0.13505 (8)	0.0250 (4)
H11	0.3061	0.6053	0.1528	0.030*
C12	0.1443 (3)	0.7442 (2)	0.09273 (8)	0.0285 (4)
H12	0.2619	0.8063	0.0813	0.034*
C13	−0.0541 (3)	0.7733 (2)	0.06721 (8)	0.0291 (4)
H13	−0.0726	0.8557	0.0385	0.035*
C14	−0.2241 (3)	0.6824 (2)	0.08370 (8)	0.0292 (4)
H14	−0.3599	0.7024	0.0663	0.035*
C15	−0.1974 (3)	0.5614 (2)	0.12572 (8)	0.0247 (4)
H15	−0.3149	0.4988	0.1368	0.030*
N1	0.2257 (2)	0.32261 (15)	0.19189 (6)	0.0193 (3)

N2	0.5455 (2)	0.21984 (17)	0.21242 (7)	0.0252 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0217 (8)	0.0153 (7)	0.0211 (7)	−0.0007 (7)	0.0028 (6)	0.0023 (6)
C2	0.0253 (8)	0.0219 (8)	0.0233 (8)	0.0021 (7)	−0.0003 (7)	0.0025 (6)
C3	0.0366 (10)	0.0225 (8)	0.0200 (8)	0.0003 (8)	0.0017 (7)	0.0004 (6)
C4	0.0348 (10)	0.0209 (8)	0.0252 (8)	0.0024 (9)	0.0092 (8)	−0.0010 (7)
C5	0.0232 (8)	0.0205 (8)	0.0316 (9)	0.0024 (7)	0.0054 (7)	0.0033 (7)
C6	0.0213 (8)	0.0187 (7)	0.0239 (7)	−0.0022 (7)	0.0019 (7)	0.0021 (6)
C7	0.0234 (8)	0.0221 (8)	0.0232 (8)	−0.0009 (7)	−0.0032 (7)	0.0001 (7)
C8	0.0177 (7)	0.0185 (7)	0.0233 (8)	0.0008 (7)	0.0023 (6)	0.0004 (6)
C9	0.0304 (9)	0.0251 (8)	0.0232 (8)	0.0040 (9)	0.0052 (9)	−0.0001 (7)
C10	0.0223 (8)	0.0190 (7)	0.0177 (7)	0.0017 (7)	0.0011 (7)	−0.0020 (6)
C11	0.0232 (9)	0.0232 (8)	0.0285 (9)	0.0030 (7)	0.0012 (7)	0.0025 (7)
C12	0.0330 (10)	0.0234 (9)	0.0290 (9)	0.0020 (8)	0.0093 (8)	0.0040 (7)
C13	0.0410 (11)	0.0255 (9)	0.0207 (7)	0.0108 (9)	0.0049 (7)	0.0027 (7)
C14	0.0294 (9)	0.0317 (9)	0.0264 (8)	0.0090 (9)	−0.0047 (8)	−0.0018 (7)
C15	0.0231 (8)	0.0253 (8)	0.0257 (8)	0.0007 (8)	−0.0004 (7)	−0.0010 (7)
N1	0.0204 (7)	0.0186 (6)	0.0189 (6)	0.0005 (6)	0.0000 (5)	−0.0001 (5)
N2	0.0234 (7)	0.0254 (7)	0.0267 (7)	0.0013 (6)	−0.0028 (6)	−0.0004 (6)

Geometric parameters (Å, °)

C1—N1	1.3858 (19)	C8—C10	1.522 (2)
C1—C2	1.391 (2)	C8—H8	1.0000
C1—C6	1.398 (2)	C9—H9A	0.9800
C2—C3	1.381 (2)	C9—H9B	0.9800
C2—H2	0.9500	C9—H9C	0.9800
C3—C4	1.402 (3)	C10—C11	1.386 (2)
C3—H3	0.9500	C10—C15	1.391 (2)
C4—C5	1.383 (3)	C11—C12	1.390 (2)
C4—H4	0.9500	C11—H11	0.9500
C5—C6	1.401 (2)	C12—C13	1.389 (3)
C5—H5	0.9500	C12—H12	0.9500
C6—N2	1.395 (2)	C13—C14	1.379 (3)
C7—N2	1.311 (2)	C13—H13	0.9500
C7—N1	1.364 (2)	C14—C15	1.393 (2)
C7—H7	0.9500	C14—H14	0.9500
C8—N1	1.469 (2)	C15—H15	0.9500
C8—C9	1.522 (2)		
N1—C1—C2	131.74 (16)	C8—C9—H9B	109.5
N1—C1—C6	105.56 (14)	H9A—C9—H9B	109.5
C2—C1—C6	122.70 (15)	C8—C9—H9C	109.5
C3—C2—C1	116.44 (16)	H9A—C9—H9C	109.5
C3—C2—H2	121.8	H9B—C9—H9C	109.5
C1—C2—H2	121.8	C11—C10—C15	119.24 (15)

C2—C3—C4	121.88 (16)	C11—C10—C8	121.71 (15)
C2—C3—H3	119.1	C15—C10—C8	118.99 (15)
C4—C3—H3	119.1	C10—C11—C12	120.53 (17)
C5—C4—C3	121.31 (16)	C10—C11—H11	119.7
C5—C4—H4	119.3	C12—C11—H11	119.7
C3—C4—H4	119.3	C13—C12—C11	119.92 (17)
C4—C5—C6	117.67 (17)	C13—C12—H12	120.0
C4—C5—H5	121.2	C11—C12—H12	120.0
C6—C5—H5	121.2	C14—C13—C12	119.86 (16)
N2—C6—C1	110.21 (14)	C14—C13—H13	120.1
N2—C6—C5	129.79 (16)	C12—C13—H13	120.1
C1—C6—C5	119.99 (16)	C13—C14—C15	120.20 (17)
N2—C7—N1	114.61 (15)	C13—C14—H14	119.9
N2—C7—H7	122.7	C15—C14—H14	119.9
N1—C7—H7	122.7	C10—C15—C14	120.25 (17)
N1—C8—C9	111.16 (14)	C10—C15—H15	119.9
N1—C8—C10	110.91 (13)	C14—C15—H15	119.9
C9—C8—C10	110.92 (13)	C7—N1—C1	105.73 (13)
N1—C8—H8	107.9	C7—N1—C8	129.94 (13)
C9—C8—H8	107.9	C1—N1—C8	124.27 (13)
C10—C8—H8	107.9	C7—N2—C6	103.88 (14)
C8—C9—H9A	109.5		
N1—C1—C2—C3	178.50 (16)	C11—C12—C13—C14	−0.4 (3)
C6—C1—C2—C3	−0.9 (2)	C12—C13—C14—C15	−0.1 (3)
C1—C2—C3—C4	0.3 (2)	C11—C10—C15—C14	0.1 (2)
C2—C3—C4—C5	0.4 (3)	C8—C10—C15—C14	177.38 (14)
C3—C4—C5—C6	−0.5 (2)	C13—C14—C15—C10	0.3 (3)
N1—C1—C6—N2	0.65 (17)	N2—C7—N1—C1	0.02 (19)
C2—C1—C6—N2	−179.85 (15)	N2—C7—N1—C8	177.34 (14)
N1—C1—C6—C5	−178.71 (14)	C2—C1—N1—C7	−179.84 (17)
C2—C1—C6—C5	0.8 (2)	C6—C1—N1—C7	−0.40 (16)
C4—C5—C6—N2	−179.32 (16)	C2—C1—N1—C8	2.6 (3)
C4—C5—C6—C1	−0.1 (2)	C6—C1—N1—C8	−177.92 (13)
N1—C8—C10—C11	−39.39 (19)	C9—C8—N1—C7	−3.7 (2)
C9—C8—C10—C11	84.65 (19)	C10—C8—N1—C7	120.19 (17)
N1—C8—C10—C15	143.39 (15)	C9—C8—N1—C1	173.17 (14)
C9—C8—C10—C15	−92.57 (18)	C10—C8—N1—C1	−62.93 (18)
C15—C10—C11—C12	−0.6 (2)	N1—C7—N2—C6	0.38 (19)
C8—C10—C11—C12	−177.81 (15)	C1—C6—N2—C7	−0.63 (17)
C10—C11—C12—C13	0.7 (3)	C5—C6—N2—C7	178.64 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···N2^{i}	1.00	2.50	3.422 (2)	152

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1

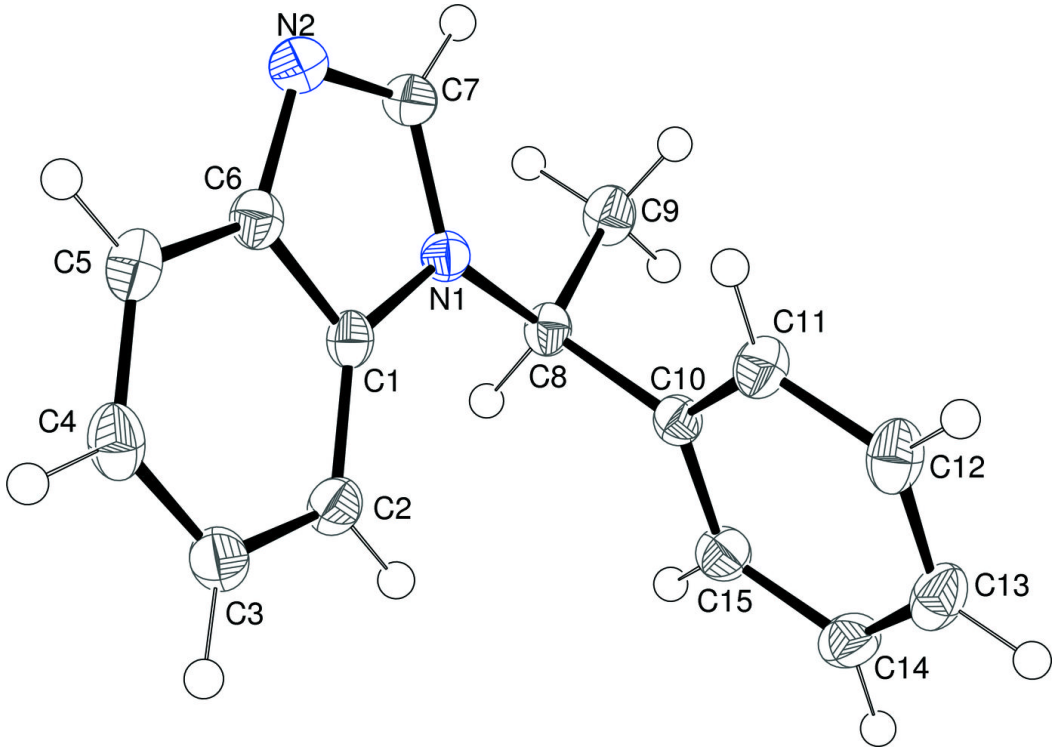

Fig. 2