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(1*S*,2*R*)-1-[(*E*)-(Thiophen-2-ylmethylidene)amino]indan-2-ol

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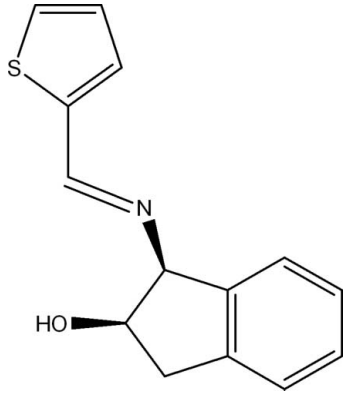
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.131; data-to-parameter ratio = 20.5.

In the title compound, $C_{14}H_{13}NOS$, the dihedral angle formed by the mean planes through the indane ring system and the thiophene ring is 85.04 (11)°. The imine bond is located in the thiophene plane [the S—C—C—N torsion angle is 0.00 (3)°] and an intramolecular O—H···N hydrogen bond is observed.

Related literature

For metal complexes containing aminoindanol ligands, see: Lee *et al.* (2007); Flores-Lopes *et al.* (2000). For metal comlexes with thiophene-type ligands, see: Jeong *et al.* (2011); Dong *et al.* (2006); Lee *et al.* (1999).



Experimental

Crystal data

$C_{14}H_{13}NOS$
M_r = 243.31
Monoclinic, $P2_1$
a = 5.8640 (2) Å
b = 13.4454 (5) Å
c = 8.0118 (3) Å
β = 92.258 (2)°
V = 631.19 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 296 K
0.25 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.943, T_{max} = 0.965
7148 measured reflections
3182 independent reflections
2848 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.131
S = 1.03
3182 reflections
155 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Absolute structure: Flack (1983), 1201 Friedel pairs
Flack parameter: 0.06 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
O—H1···N	0.82	2.22	2.682 (3)	116

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2077).

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supporting information

Acta Cryst. (2012). E**68**, o2568 [https://doi.org/10.1107/S1600536812032783]

(1*S*,2*R*)-1-[(*E*)-(Thiophen-2-ylmethylidene)amino]indan-2-ol

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S1. Comment

Multidentate ligands having thiophene groups have received a great attention due to their unique binding abilities (Jeong *et al.*, 2011; Dong *et al.*, 2006; Lee *et al.*, 1999). Aminoindaol type ligands have been also extensively used as chiral chelating ligands (Lee *et al.*, 2007; Flores-Lopes *et al.*, 2000). As a part of our ongoing project on the synthesis of new ONS-type tridentate monoanionic chelating ligands, the title compound was synthesized by the reaction of 2-thiophene carboxaldehyde with (1*S*,2*R*)-(-)-*cis*-amino-2-indanol and its crystal structure is reported herein.

In the title compound (Fig. 1), the C7 carbon atom is displaced by 0.450 (2) Å from the mean plane defined by the C6/C8–C14 atoms of the indane ring system. The dihedral angle formed by the mean planes through the indane ring system and the thiophene is 85.04 (11) °. The molecular conformation is stabilized by an intramolecular O—H···N hydrogen bond (Table 1). The absolute configuration is assigned on the basis of the Flack parameter, which is consistent with the known configuration of the indanol employed in the synthesis.

S2. Experimental

A mixture of (1*S*,2*R*)-(-)-amino-2-indanol (0.149 g,1 mmol) and 2-thiophene carboxaldehyde (0.112 g,1 mmol) was stirred in ethanol for 24 h. The residue, obtained by removing the solvent under vacuum, was recrystallized in dichloromethane. The desired product was isolated as white crystals after the solution remained at -20 °C in a refrigerator for a few days (yield 80%, 0.195 g).

S3. Refinement

The H-atoms were included in calculated positions and treated as riding atoms: U_{iso}(H) = 1.2Ueq(parent C-atom),U_{iso}(H) = 1.5Ueq(parent O-atom).

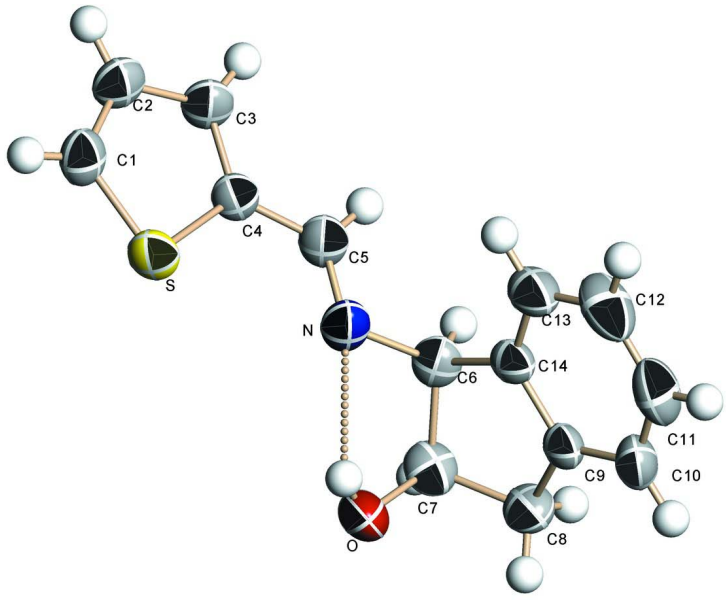

Figure 1

Molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as spheres of arbitrary radius. Hydrogen bonds are drawn as dashed lines.

(1*S*,2*R*)-1-[(*E*)-(Thiophen-2-ylmethylidene)amino]indan-2-ol

Crystal data

$C_{14}H_{13}NOS$
$M_r = 243.31$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 5.8640\ (2)$ Å
$b = 13.4454\ (5)$ Å
$c = 8.0118\ (3)$ Å
$\beta = 92.258\ (2)°$
$V = 631.19\ (4)$ Å^3
$Z = 2$
$F(000) = 256$
$D_x = 1.280$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5424 reflections
$\theta = 2.5–30.4°$
$\mu = 0.24$ mm^{-1}
$T = 296$ K
Block, white
0.25 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.943$, $T_{max} = 0.965$
7148 measured reflections
3182 independent reflections
2848 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 30.7°$, $\theta_{min} = 2.5°$
$h = -8\rightarrow7$
$k = -15\rightarrow18$
$l = -11\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.131$
$S = 1.03$
3182 reflections
155 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Absolute structure: Flack (1983), 1201 Friedel pairs
Absolute structure parameter: 0.06 (8)

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O	0.3762 (3)	0.41344 (15)	0.6763 (2)	0.0694 (4)
H1	0.3962	0.4736	0.6845	0.104*
S	0.84192 (7)	0.69970 (5)	0.55448 (6)	0.05798 (16)
C9	0.3596 (3)	0.40337 (14)	1.0537 (2)	0.0437 (4)
C14	0.5379 (3)	0.46986 (12)	1.0333 (2)	0.0431 (3)
C4	1.0148 (3)	0.64078 (15)	0.7010 (2)	0.0473 (4)
C13	0.5668 (4)	0.55083 (16)	1.1369 (3)	0.0602 (5)
H13	0.6866	0.5950	1.1232	0.072*
C3	1.2263 (3)	0.68631 (19)	0.7167 (3)	0.0552 (5)
H3	1.3433	0.6657	0.7904	0.066*
C1	1.0474 (3)	0.78383 (18)	0.5133 (3)	0.0567 (5)
H1A	1.0286	0.8349	0.4356	0.068*
C5	0.9397 (3)	0.55622 (17)	0.7985 (3)	0.0524 (4)
H5	1.0416	0.5274	0.8761	0.063*
C6	0.6804 (3)	0.43819 (15)	0.8891 (3)	0.0508 (4)
H6	0.8190	0.4043	0.9312	0.061*
C2	1.2422 (3)	0.76835 (17)	0.6062 (3)	0.0573 (5)
H2	1.3724	0.8073	0.5985	0.069*
C8	0.3710 (4)	0.32062 (16)	0.9292 (3)	0.0570 (5)
H8A	0.2204	0.3041	0.8830	0.068*
H8B	0.4395	0.2616	0.9794	0.068*
C7	0.5206 (4)	0.36346 (16)	0.7957 (3)	0.0574 (5)
H7	0.6085	0.3110	0.7428	0.069*

C12	0.4134 (6)	0.5654 (2)	1.2626 (3)	0.0789 (8)
H12	0.4314	0.6194	1.3345	0.095*
C10	0.2064 (4)	0.4177 (2)	1.1781 (3)	0.0594 (5)
H10	0.0874	0.3732	1.1925	0.071*
C11	0.2347 (5)	0.5002 (3)	1.2812 (3)	0.0742 (7)
H11	0.1313	0.5117	1.3641	0.089*
N	0.7401 (3)	0.52068 (15)	0.7810 (2)	0.0549 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O	0.0800 (10)	0.0776 (11)	0.0494 (8)	−0.0161 (9)	−0.0110 (7)	0.0048 (8)
S	0.0389 (2)	0.0805 (3)	0.0542 (3)	0.0031 (2)	−0.00272 (16)	0.0050 (3)
C9	0.0500 (8)	0.0434 (8)	0.0370 (8)	0.0001 (6)	−0.0051 (6)	0.0072 (6)
C14	0.0453 (8)	0.0416 (8)	0.0418 (8)	0.0025 (6)	−0.0075 (6)	0.0049 (7)
C4	0.0335 (7)	0.0623 (10)	0.0462 (9)	0.0047 (6)	0.0029 (6)	0.0021 (8)
C13	0.0775 (14)	0.0474 (10)	0.0549 (12)	−0.0071 (9)	−0.0102 (10)	0.0007 (9)
C3	0.0331 (6)	0.0706 (13)	0.0619 (11)	0.0030 (8)	0.0003 (6)	0.0081 (10)
C1	0.0487 (9)	0.0717 (12)	0.0505 (11)	0.0071 (9)	0.0133 (8)	0.0074 (9)
C5	0.0376 (7)	0.0647 (12)	0.0548 (10)	0.0089 (7)	0.0015 (7)	0.0091 (9)
C6	0.0395 (8)	0.0552 (10)	0.0576 (11)	0.0098 (7)	0.0010 (7)	0.0069 (8)
C2	0.0385 (8)	0.0706 (13)	0.0634 (12)	−0.0013 (8)	0.0105 (8)	0.0034 (10)
C8	0.0693 (12)	0.0416 (9)	0.0596 (13)	−0.0063 (8)	−0.0029 (9)	0.0023 (8)
C7	0.0661 (12)	0.0512 (10)	0.0552 (11)	0.0080 (8)	0.0043 (9)	−0.0086 (9)
C12	0.125 (2)	0.0626 (15)	0.0490 (13)	0.0113 (14)	−0.0034 (13)	−0.0128 (11)
C10	0.0629 (12)	0.0736 (14)	0.0417 (10)	−0.0035 (9)	0.0018 (8)	0.0130 (9)
C11	0.0851 (17)	0.0953 (19)	0.0427 (11)	0.0132 (14)	0.0091 (10)	0.0013 (12)
N	0.0383 (7)	0.0697 (11)	0.0569 (10)	0.0033 (7)	0.0031 (6)	0.0104 (8)

Geometric parameters (Å, º)

O—C7	1.421 (3)	C1—H1A	0.9300
O—H1	0.8200	C5—N	1.267 (3)
S—C1	1.695 (2)	C5—H5	0.9300
S—C4	1.7143 (19)	C6—N	1.458 (3)
C9—C10	1.381 (3)	C6—C7	1.546 (3)
C9—C14	1.390 (2)	C6—H6	0.9800
C9—C8	1.498 (3)	C2—H2	0.9300
C14—C13	1.376 (3)	C8—C7	1.523 (3)
C14—C6	1.513 (3)	C8—H8A	0.9700
C4—C3	1.384 (3)	C8—H8B	0.9700
C4—C5	1.457 (3)	C7—H7	0.9800
C13—C12	1.390 (4)	C12—C11	1.379 (5)
C13—H13	0.9300	C12—H12	0.9300
C3—C2	1.420 (3)	C10—C11	1.390 (4)
C3—H3	0.9300	C10—H10	0.9300
C1—C2	1.355 (3)	C11—H11	0.9300

C7—O—H1	109.5	C14—C6—H6	110.1
C1—S—C4	92.06 (10)	C7—C6—H6	110.1
C10—C9—C14	120.60 (19)	C1—C2—C3	112.79 (18)
C10—C9—C8	129.15 (19)	C1—C2—H2	123.6
C14—C9—C8	110.23 (16)	C3—C2—H2	123.6
C13—C14—C9	120.86 (19)	C9—C8—C7	103.23 (16)
C13—C14—C6	128.70 (18)	C9—C8—H8A	111.1
C9—C14—C6	110.44 (16)	C7—C8—H8A	111.1
C3—C4—C5	125.80 (18)	C9—C8—H8B	111.1
C3—C4—S	111.18 (15)	C7—C8—H8B	111.1
C5—C4—S	122.99 (14)	H8A—C8—H8B	109.1
C14—C13—C12	118.8 (2)	O—C7—C8	107.87 (19)
C14—C13—H13	120.6	O—C7—C6	110.60 (17)
C12—C13—H13	120.6	C8—C7—C6	105.13 (18)
C4—C3—C2	111.57 (17)	O—C7—H7	111.0
C4—C3—H3	124.2	C8—C7—H7	111.0
C2—C3—H3	124.2	C6—C7—H7	111.0
C2—C1—S	112.40 (17)	C11—C12—C13	120.3 (2)
C2—C1—H1A	123.8	C11—C12—H12	119.8
S—C1—H1A	123.8	C13—C12—H12	119.8
N—C5—C4	122.17 (19)	C9—C10—C11	118.3 (2)
N—C5—H5	118.9	C9—C10—H10	120.9
C4—C5—H5	118.9	C11—C10—H10	120.9
N—C6—C14	113.08 (16)	C12—C11—C10	121.1 (2)
N—C6—C7	111.23 (18)	C12—C11—H11	119.4
C14—C6—C7	102.12 (15)	C10—C11—H11	119.4
N—C6—H6	110.1	C5—N—C6	117.62 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O—H1···N	0.82	2.22	2.682 (3)	116