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# 2-[(Indan-1-ylidene)amino]ethanol

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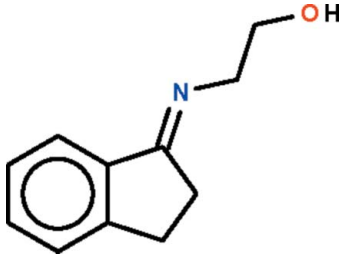
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.037; $wR$ factor = 0.099; data-to-parameter ratio = 14.3.

The five-membed ring of the title compound, $C_{11}H_{13}NO$, that is fused with the aromatic ring is approximately planar (r.m.s. deviation = 0.037 Å) despite the presence of the $sp^3$-hybridized ethylene linkage. The hydroxy group of the N-bound hydroxyethyl chain serves as hydrogen-bond donor to the azomethine N atom of an adjacent molecule, generating a hydrogen-bonded $C_2$-symmetric dimer.

## Related literature

The related $C_{13}H_{13}NO$ amine is a reagent in the synthesis of pharmaceuticals, see: Stange *et al.* (1957).




## Experimental

### Crystal data

$C_{11}H_{13}NO$
$M_r$ = 175.22
Monoclinic, $C2/c$
$a$ = 16.0207 (4) Å
$b$ = 9.2002 (2) Å
$c$ = 13.0600 (3) Å
$\beta$ = 112.855 (3)°
$V$ = 1773.83 (7) Å$^3$
$Z$ = 8
Cu $K\alpha$ radiation
$\mu$ = 0.67 mm$^{-1}$
$T$ = 100 K
0.30 × 0.30 × 0.10 mm

### Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.825, $T_{max}$ = 0.937
3090 measured reflections
1745 independent reflections
1590 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.015

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.099
$S$ = 1.02
1745 reflections
122 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N1$^{i}$ | 0.91 (2) | 1.91 (2) | 2.820 (1) | 173 (2) |

Symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2010); 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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank King Abdulaziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5608).

## References

Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stange, K., Friederich, H. & Amann, A. (1957). Ger. Patent 955497, 19570103.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

# supporting information

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## 2-[(Indan-1-ylidene)amino]ethanol

**Abdulrahman O. Al-Youbi, Abdullah M. Asiri, Hassan M. Faidallah, Khalid A. Alamry and Seik Weng Ng**

### S1. Comment

A enormously large number of Schiff base derivatives of aldehydes and ketones have been synthesized; however, 1-indanone represents an anomaly as only few have been reported. In the 2-aminoethanol derivative (Scheme I), the five-membed cyclohexene ring is planar despite the presence of $sp^3$-hybridized ethylene linkage molecule (Fig. 1). The hydroxy group of the *N*-bound hydroxyethyl chain serves as hydrogen-bond donor to the azomethine N atom of an adjacent molecule to generate a hydrogen-bonded dinuclear molecule (Table 1). However, there is no significant $\pi$ interaction of the rings as the distances between them exceed 3.5 Å (Fig. 2). The compound has not been reported in the chemical literature; on the other hand, the corresponding reduced amine is a reagent for the synthesis of pharmaceuticals (Stange *et al.*, 1957).

### S2. Experimental

A mixture of 2-amino ethanol (0.6 g, 10 mmol) and 1-indanone (1.3 g, 10 mmol) in dry benzene (50 ml) was refluxed in a Dean-Stark apparatus until no more water was collected (in about 2 h). The solvent was then removed under reduced pressure and the residue treated with methanol. The solid which separated out was recystalized from ethanol to give colorless, 418–419 K.

### S3. Refinement

Carbon bound H-atoms were placed in calculated positions [C–H 0.95 to 0.99 Å, $U_{iso}$(H) 1.2$U_{eq}$(C)] and were included in the refinement in the riding model approximation.

The hydroxy H-atom was located in a difference Fouier map and was freely refined.

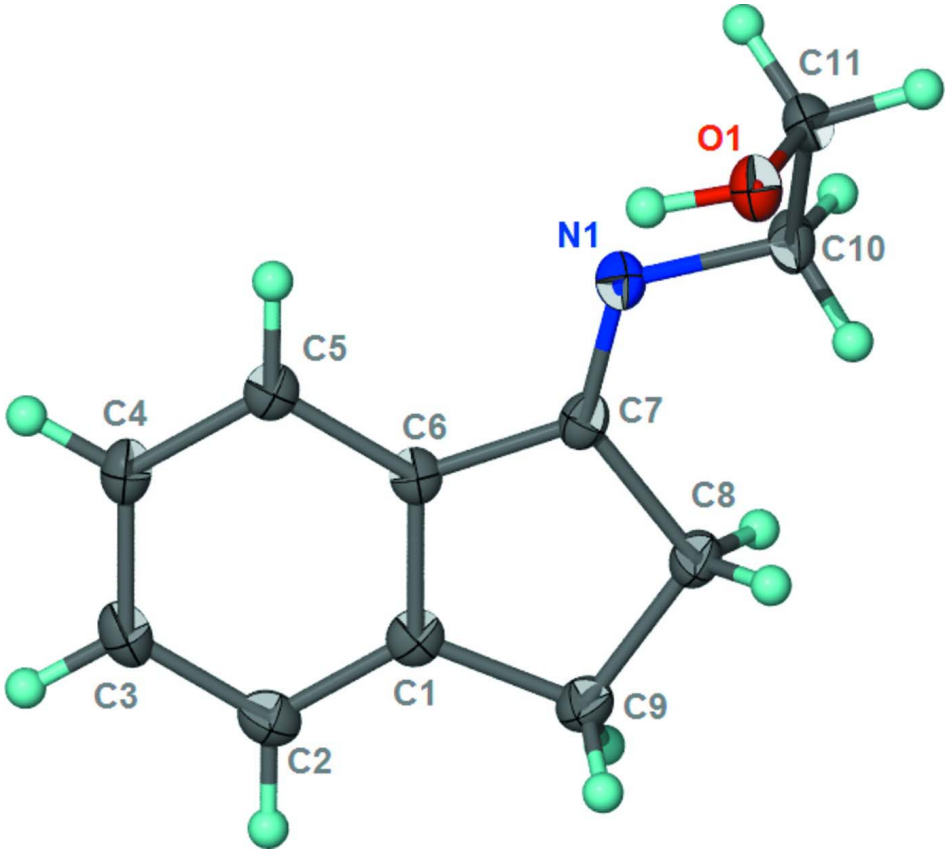


**Figure 1**

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{13}H_{11}NO$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

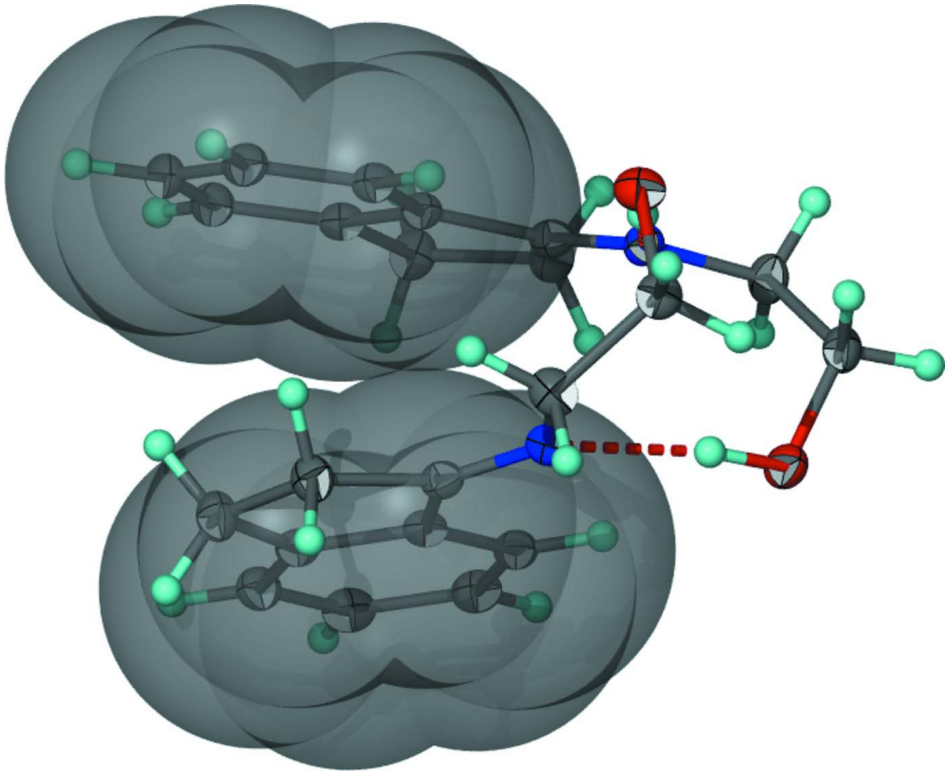

**Figure 2**

Hydrogen-bonded dimer. The atoms of the aromatic rings are shown with their van der Waals surfaces.

### 2-[(Indan-1-ylidene)amino]ethanol

*Crystal data*

$C_{11}H_{13}NO$
$M_r = 175.22$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 16.0207\ (4)$ Å
$b = 9.2002\ (2)$ Å
$c = 13.0600\ (3)$ Å
$\beta = 112.855\ (3)°$
$V = 1773.83\ (7)$ Å$^3$
$Z = 8$

$F(000) = 752$
$D_x = 1.312$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 1977 reflections
$\theta = 3.7–74.2°$
$\mu = 0.67$ mm$^{-1}$
$T = 100$ K
Prism, colorless
0.30 × 0.30 × 0.10 mm

*Data collection*

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)

$T_{min} = 0.825$, $T_{max} = 0.937$
3090 measured reflections
1745 independent reflections
1590 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 74.4°$, $\theta_{min} = 5.7°$
$h = -19\rightarrow19$
$k = -11\rightarrow6$
$l = -15\rightarrow16$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.099$
$S = 1.02$
1745 reflections
122 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2 + 1.1159P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å$^{-3}$
$\Delta\rho_{min} = -0.21$ e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.61199 (6) | 0.25279 (9) | 0.23182 (7) | 0.0186 (2) |
| H1 | 0.5586 (14) | 0.303 (2) | 0.2000 (16) | 0.051 (6)* |
| N1 | 0.54795 (6) | 0.41152 (11) | 0.38232 (7) | 0.0155 (2) |
| C1 | 0.50616 (8) | 0.78897 (13) | 0.39934 (9) | 0.0162 (3) |
| C2 | 0.44473 (8) | 0.90379 (13) | 0.36833 (10) | 0.0186 (3) |
| H2 | 0.4646 | 1.0007 | 0.3891 | 0.022* |
| C3 | 0.35384 (8) | 0.87441 (13) | 0.30649 (10) | 0.0194 (3) |
| H3 | 0.3114 | 0.9521 | 0.2851 | 0.023* |
| C4 | 0.32389 (8) | 0.73221 (13) | 0.27531 (9) | 0.0180 (3) |
| H4 | 0.2615 | 0.7139 | 0.2334 | 0.022* |
| C5 | 0.38514 (8) | 0.61760 (13) | 0.30546 (9) | 0.0160 (3) |
| H5 | 0.3653 | 0.5209 | 0.2840 | 0.019* |
| C6 | 0.47636 (7) | 0.64727 (12) | 0.36786 (9) | 0.0148 (3) |
| C7 | 0.55414 (7) | 0.54679 (13) | 0.40624 (9) | 0.0147 (3) |
| C8 | 0.63802 (7) | 0.63476 (13) | 0.47441 (9) | 0.0174 (3) |
| H8A | 0.6859 | 0.6219 | 0.4450 | 0.021* |
| H8B | 0.6620 | 0.6034 | 0.5531 | 0.021* |
| C9 | 0.60731 (8) | 0.79464 (13) | 0.46423 (10) | 0.0192 (3) |
| H9A | 0.6218 | 0.8381 | 0.5385 | 0.023* |
| H9B | 0.6372 | 0.8525 | 0.4242 | 0.023* |
| C10 | 0.63052 (8) | 0.32330 (13) | 0.42013 (9) | 0.0181 (3) |
| H10A | 0.6415 | 0.2820 | 0.4942 | 0.022* |
| H10B | 0.6830 | 0.3850 | 0.4268 | 0.022* |
| C11 | 0.62087 (8) | 0.20122 (12) | 0.33805 (9) | 0.0173 (3) |
| H11A | 0.6747 | 0.1373 | 0.3680 | 0.021* |
| H11B | 0.5670 | 0.1423 | 0.3299 | 0.021* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0162 (4) | 0.0219 (4) | 0.0178 (4) | 0.0038 (3) | 0.0067 (3) | 0.0012 (3) |
| N1 | 0.0144 (5) | 0.0173 (5) | 0.0142 (5) | 0.0019 (4) | 0.0047 (4) | 0.0002 (4) |
| C1 | 0.0172 (6) | 0.0184 (6) | 0.0147 (5) | −0.0006 (4) | 0.0080 (4) | −0.0002 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.0223 (6) | 0.0158 (5) | 0.0194 (6) | 0.0006 (5) | 0.0102 (5) | 0.0001 (4) |
| C3 | 0.0198 (6) | 0.0199 (6) | 0.0197 (6) | 0.0062 (5) | 0.0090 (5) | 0.0043 (5) |
| C4 | 0.0144 (5) | 0.0230 (6) | 0.0163 (5) | 0.0023 (5) | 0.0055 (4) | 0.0018 (4) |
| C5 | 0.0158 (6) | 0.0182 (6) | 0.0147 (5) | −0.0002 (4) | 0.0066 (4) | −0.0003 (4) |
| C6 | 0.0153 (6) | 0.0168 (6) | 0.0131 (5) | 0.0013 (4) | 0.0064 (4) | 0.0005 (4) |
| C7 | 0.0128 (5) | 0.0191 (6) | 0.0120 (5) | −0.0007 (4) | 0.0044 (4) | 0.0000 (4) |
| C8 | 0.0139 (5) | 0.0187 (6) | 0.0171 (5) | −0.0007 (4) | 0.0033 (4) | −0.0014 (4) |
| C9 | 0.0165 (6) | 0.0174 (6) | 0.0222 (6) | −0.0017 (4) | 0.0058 (5) | −0.0031 (5) |
| C10 | 0.0144 (5) | 0.0197 (6) | 0.0166 (6) | 0.0041 (4) | 0.0020 (4) | 0.0005 (4) |
| C11 | 0.0159 (5) | 0.0161 (5) | 0.0191 (6) | 0.0028 (4) | 0.0058 (4) | 0.0018 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C11 | 1.4201 (14) | C5—H5 | 0.9500 |
| O1—H1 | 0.91 (2) | C6—C7 | 1.4742 (15) |
| N1—C7 | 1.2776 (15) | C7—C8 | 1.5245 (15) |
| N1—C10 | 1.4646 (14) | C8—C9 | 1.5403 (16) |
| C1—C2 | 1.3924 (16) | C8—H8A | 0.9900 |
| C1—C6 | 1.3943 (16) | C8—H8B | 0.9900 |
| C1—C9 | 1.5101 (16) | C9—H9A | 0.9900 |
| C2—C3 | 1.3900 (16) | C9—H9B | 0.9900 |
| C2—H2 | 0.9500 | C10—C11 | 1.5185 (16) |
| C3—C4 | 1.3985 (17) | C10—H10A | 0.9900 |
| C3—H3 | 0.9500 | C10—H10B | 0.9900 |
| C4—C5 | 1.3890 (16) | C11—H11A | 0.9900 |
| C4—H4 | 0.9500 | C11—H11B | 0.9900 |
| C5—C6 | 1.3962 (15) | | |
| | | | |
| C11—O1—H1 | 109.4 (12) | C7—C8—H8A | 110.5 |
| C7—N1—C10 | 118.90 (10) | C9—C8—H8A | 110.5 |
| C2—C1—C6 | 120.08 (11) | C7—C8—H8B | 110.5 |
| C2—C1—C9 | 128.34 (11) | C9—C8—H8B | 110.5 |
| C6—C1—C9 | 111.57 (10) | H8A—C8—H8B | 108.7 |
| C3—C2—C1 | 118.95 (11) | C1—C9—C8 | 104.63 (9) |
| C3—C2—H2 | 120.5 | C1—C9—H9A | 110.8 |
| C1—C2—H2 | 120.5 | C8—C9—H9A | 110.8 |
| C2—C3—C4 | 120.97 (11) | C1—C9—H9B | 110.8 |
| C2—C3—H3 | 119.5 | C8—C9—H9B | 110.8 |
| C4—C3—H3 | 119.5 | H9A—C9—H9B | 108.9 |
| C5—C4—C3 | 120.20 (11) | N1—C10—C11 | 109.93 (9) |
| C5—C4—H4 | 119.9 | N1—C10—H10A | 109.7 |
| C3—C4—H4 | 119.9 | C11—C10—H10A | 109.7 |
| C4—C5—C6 | 118.76 (11) | N1—C10—H10B | 109.7 |
| C4—C5—H5 | 120.6 | C11—C10—H10B | 109.7 |
| C6—C5—H5 | 120.6 | H10A—C10—H10B | 108.2 |
| C1—C6—C5 | 121.05 (11) | O1—C11—C10 | 112.74 (9) |
| C1—C6—C7 | 109.80 (10) | O1—C11—H11A | 109.0 |
| C5—C6—C7 | 129.11 (11) | C10—C11—H11A | 109.0 |

| | | | |
|---|---|---|---|
| N1—C7—C6 | 123.55 (10) | O1—C11—H11B | 109.0 |
| N1—C7—C8 | 128.83 (10) | C10—C11—H11B | 109.0 |
| C6—C7—C8 | 107.61 (10) | H11A—C11—H11B | 107.8 |
| C7—C8—C9 | 106.09 (9) | | |
| | | | |
| C6—C1—C2—C3 | 0.39 (17) | C10—N1—C7—C8 | −2.07 (17) |
| C9—C1—C2—C3 | 178.90 (11) | C1—C6—C7—N1 | −174.79 (10) |
| C1—C2—C3—C4 | −0.12 (17) | C5—C6—C7—N1 | 2.73 (18) |
| C2—C3—C4—C5 | −0.35 (18) | C1—C6—C7—C8 | 4.31 (12) |
| C3—C4—C5—C6 | 0.53 (16) | C5—C6—C7—C8 | −178.17 (11) |
| C2—C1—C6—C5 | −0.20 (17) | N1—C7—C8—C9 | 173.44 (11) |
| C9—C1—C6—C5 | −178.95 (10) | C6—C7—C8—C9 | −5.60 (12) |
| C2—C1—C6—C7 | 177.55 (10) | C2—C1—C9—C8 | 179.04 (11) |
| C9—C1—C6—C7 | −1.19 (13) | C6—C1—C9—C8 | −2.35 (13) |
| C4—C5—C6—C1 | −0.26 (16) | C7—C8—C9—C1 | 4.78 (12) |
| C4—C5—C6—C7 | −177.54 (10) | C7—N1—C10—C11 | −148.98 (10) |
| C10—N1—C7—C6 | 176.83 (10) | N1—C10—C11—O1 | 63.93 (12) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N1$^{i}$ | 0.91 (2) | 1.91 (2) | 2.820 (1) | 173 (2) |

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.