

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

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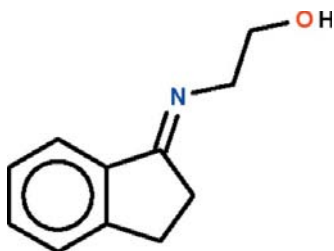
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.037; wR factor = 0.099; data-to-parameter ratio = 14.3.

The five-membered ring of the title compound, $\text{C}_{11}\text{H}_{13}\text{NO}$, 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 $\text{C}_{13}\text{H}_{13}\text{NO}$ amine is a reagent in the synthesis of pharmaceuticals, see: Stange *et al.* (1957).



Experimental

Crystal data

 $\text{C}_{11}\text{H}_{13}\text{NO}$
 $M_r = 175.22$
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) Å³
 $Z = 8$
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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.015$

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, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{N1}^{\dagger}$	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).

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

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