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2-(Anilinomethyl)phenol

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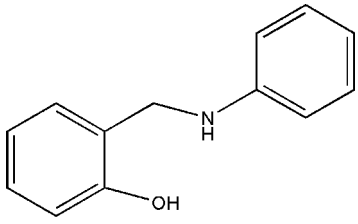
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.108; data-to-parameter ratio = 13.8.

In the title compound, $C_{13}H_{13}NO$, which was synthesized by the reduction of 2-(phenyliminomethyl)phenol, the dihedral angle between the two benzene ring planes is 71.08 (4)°. The crystal structure exhibits the formation of centrosymmetric dimers by intermolecular O—H···N hydrogen bonds, characterized by an $R_2^2(12)$ pattern. These dimers are further connected by N—H···O hydrogen bonds.

Related literature

For related literature, see: Aguiari *et al.* (1992); Arod *et al.* (2005); Baker *et al.* (1992); Jeevanandam *et al.*(2000); Noda (1959).



Experimental

Crystal data

$C_{13}H_{13}NO$
M_r = 199.24
Triclinic, $P\overline{1}$
a = 5.5911 (16) Å
b = 7.932 (2) Å
c = 11.803 (3) Å
α = 90.649 (5)°
β = 91.985 (4)°
γ = 90.323 (5)°
V = 523.1 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.45 × 0.08 × 0.06 mm

Data collection

Bruker SMART APEX detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.965, T_{max} = 0.989
3981 measured reflections
1943 independent reflections
1632 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.108
S = 1.07
1943 reflections
141 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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}	0.82	1.98	2.7871 (16)	170
N1—H1A···O1^{ii}	0.864 (16)	2.233 (16)	3.0770 (17)	165.8 (13)

Symmetry codes: (i) $-x+2, -y+1, -z+2$; (ii) $x-1, y, z$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2613).

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supplementary materials

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2-(Anilinomethyl)phenol

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Comment

The structure of 2-(phenyliminomethyl)phenol is known (Arod *et al.*, 2005). We report herein the crystal structure of its reductive product which is a bidentate ligand (Baker *et al.*, 1992) (Fig. 1).

The bond lengths and angles are within normal ranges (Aguiari *et al.*, 1992; Jeevanandam *et al.*, 2000). The dihedral angle between the two phenyl ring planes is 71.08 (4)°. Centro-symmetric dimers are formed by intermolecular O—H···N hydrogen bonds characterized by an $R_2^2(12)$ pattern, which are further connected by N—H···O hydrogen bonds (Table 1).

Experimental

The title compound was synthesized by the reaction of 2-(phenyliminomethyl)phenol (1.97 g, 10 mmol) with $NaBH_4$ (0.38 g, 10 mmol) in 60 ml me thanol according to the reported method (Noda, 1959). Crystals were obtained from an ethanolic (95%) solution by slow evaporation at room temperature.

Refinement

H atoms bonded to O and C were placed at calculated positions and were included in the refinement in the riding-model approximation, with C—H = 0.93 Å and for aromatic H atoms, C—H = 0.97 Å for methylene H atoms, O—H = 0.82Å and U_{iso}(H) = 1.2Ueq(C). The H atom on N atom was freely refined.

Figures

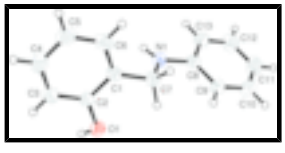

Fig. 1. The structure of (I), with displacement ellipsoids are drawn at the 30% probability level.

2-(Anilinomethyl)phenol

Crystal data

$C_{13}H_{13}NO$	$Z = 2$
$M_r = 199.24$	$F_{000} = 212$
Triclinic, $P\bar{1}$	$D_x = 1.265$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.5911$ (16) Å	Cell parameters from 1673 reflections
$b = 7.932$ (2) Å	$\theta = 2.6$–$27.2°$

c = 11.803 (3) Å	μ = 0.08 mm^{-1}
α = 90.649 (5)º	T = 295 (2) K
β = 91.985 (4)º	Prism, colorless
γ = 90.323 (5)º	0.45 × 0.08 × 0.06 mm
V = 523.1 (2) Å^3	

Data collection

Bruker SMART APEX detector diffractometer	1943 independent reflections
Radiation source: fine-focus sealed tube	1632 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017
T = 295(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$h = -6 \rightarrow 6$
T_{min} = 0.965, T_{max} = 0.989	$k = -9 \rightarrow 9$
3981 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.041	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.108	$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2 + 0.0635P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
1943 reflections	$\Delta\rho_{max}$ = 0.14 e Å^{-3}
141 parameters	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
H1A	0.524 (3)	0.7013 (18)	0.9462 (12)	0.043 (4)*
N1	0.6501 (2)	0.70555 (13)	0.90607 (9)	0.0385 (3)
O1	1.20706 (16)	0.62179 (11)	1.04289 (7)	0.0440 (3)
H1	1.2523	0.5298	1.0659	0.066*
C1	0.8734 (2)	0.79374 (16)	1.08012 (11)	0.0391 (3)
C2	1.0614 (2)	0.69432 (15)	1.12069 (10)	0.0360 (3)
C3	1.1025 (2)	0.67500 (18)	1.23582 (11)	0.0452 (3)
H3	1.2296	0.6095	1.2623	0.054*
C4	0.9552 (3)	0.7527 (2)	1.31168 (12)	0.0532 (4)
H4	0.9828	0.7387	1.3891	0.064*
C5	0.7681 (3)	0.8508 (2)	1.27337 (13)	0.0568 (4)
H5	0.6687	0.9030	1.3245	0.068*
C6	0.7296 (3)	0.87091 (19)	1.15865 (13)	0.0511 (4)
H6	0.6036	0.9381	1.1330	0.061*
C7	0.8315 (2)	0.82149 (17)	0.95536 (11)	0.0431 (3)
H7A	0.7802	0.9367	0.9433	0.052*
H7B	0.9806	0.8057	0.9170	0.052*
C8	0.5870 (2)	0.72473 (15)	0.78965 (11)	0.0382 (3)
C9	0.7269 (3)	0.81622 (19)	0.71694 (12)	0.0484 (4)
H9	0.8623	0.8735	0.7451	0.058*
C10	0.6651 (3)	0.8221 (2)	0.60285 (13)	0.0601 (4)
H10	0.7602	0.8832	0.5547	0.072*
C11	0.4659 (3)	0.7395 (2)	0.55931 (13)	0.0643 (5)
H11	0.4264	0.7436	0.4822	0.077*
C12	0.3253 (3)	0.6506 (2)	0.63132 (14)	0.0633 (5)
H12	0.1889	0.5952	0.6026	0.076*
C13	0.3841 (3)	0.64261 (19)	0.74551 (12)	0.0506 (4)
H13	0.2874	0.5819	0.7932	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0351 (6)	0.0424 (6)	0.0382 (6)	0.0004 (5)	0.0039 (5)	0.0043 (5)
O1	0.0447 (6)	0.0436 (5)	0.0445 (5)	0.0068 (4)	0.0089 (4)	0.0043 (4)
C1	0.0363 (7)	0.0364 (7)	0.0443 (7)	−0.0025 (5)	−0.0008 (5)	0.0009 (5)
C2	0.0342 (7)	0.0333 (6)	0.0407 (7)	−0.0037 (5)	0.0034 (5)	−0.0006 (5)
C3	0.0437 (8)	0.0477 (8)	0.0439 (8)	0.0024 (6)	−0.0041 (6)	0.0022 (6)
C4	0.0596 (10)	0.0618 (9)	0.0381 (7)	−0.0005 (7)	0.0012 (7)	−0.0063 (7)
C5	0.0555 (9)	0.0622 (10)	0.0533 (9)	0.0066 (8)	0.0117 (7)	−0.0125 (7)
C6	0.0433 (8)	0.0513 (8)	0.0587 (9)	0.0104 (6)	0.0009 (7)	−0.0016 (7)
C7	0.0405 (7)	0.0415 (7)	0.0471 (8)	−0.0010 (6)	−0.0021 (6)	0.0077 (6)
C8	0.0388 (7)	0.0374 (7)	0.0385 (7)	0.0086 (5)	0.0032 (5)	0.0019 (5)
C9	0.0445 (8)	0.0562 (9)	0.0446 (8)	−0.0005 (6)	0.0033 (6)	0.0058 (6)
C10	0.0632 (10)	0.0731 (11)	0.0450 (9)	0.0025 (8)	0.0103 (7)	0.0109 (7)

C11	0.0764 (12)	0.0783 (11)	0.0378 (8)	0.0056 (9)	−0.0038 (8)	0.0015 (7)
C12	0.0626 (10)	0.0726 (11)	0.0537 (9)	−0.0068 (8)	−0.0116 (8)	−0.0040 (8)
C13	0.0490 (9)	0.0543 (9)	0.0483 (8)	−0.0050 (7)	0.0000 (6)	0.0024 (6)

Geometric parameters (Å, °)

N1—C8	1.4168 (17)	C6—H6	0.9300
N1—C7	1.4663 (17)	C7—H7A	0.9700
N1—H1A	0.861 (16)	C7—H7B	0.9700
O1—C2	1.3722 (15)	C8—C13	1.3878 (19)
O1—H1	0.8200	C8—C9	1.3890 (19)
C1—C6	1.3874 (19)	C9—C10	1.380 (2)
C1—C2	1.3923 (19)	C9—H9	0.9300
C1—C7	1.5019 (18)	C10—C11	1.370 (2)
C2—C3	1.3806 (19)	C10—H10	0.9300
C3—C4	1.380 (2)	C11—C12	1.376 (2)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.374 (2)	C12—C13	1.379 (2)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.375 (2)	C13—H13	0.9300
C5—H5	0.9300		
C8—N1—C7	117.13 (11)	N1—C7—H7A	109.2
C8—N1—H1A	111.0 (9)	C1—C7—H7A	109.2
C7—N1—H1A	111.9 (10)	N1—C7—H7B	109.2
C2—O1—H1	109.5	C1—C7—H7B	109.2
C6—C1—C2	117.99 (12)	H7A—C7—H7B	107.9
C6—C1—C7	120.76 (12)	C13—C8—C9	118.75 (13)
C2—C1—C7	121.23 (12)	C13—C8—N1	118.78 (12)
O1—C2—C3	121.68 (12)	C9—C8—N1	122.39 (12)
O1—C2—C1	117.82 (11)	C10—C9—C8	120.00 (14)
C3—C2—C1	120.47 (12)	C10—C9—H9	120.0
C4—C3—C2	120.10 (13)	C8—C9—H9	120.0
C4—C3—H3	119.9	C11—C10—C9	121.12 (15)
C2—C3—H3	119.9	C11—C10—H10	119.4
C5—C4—C3	120.34 (14)	C9—C10—H10	119.4
C5—C4—H4	119.8	C10—C11—C12	119.03 (15)
C3—C4—H4	119.8	C10—C11—H11	120.5
C4—C5—C6	119.28 (14)	C12—C11—H11	120.5
C4—C5—H5	120.4	C11—C12—C13	120.81 (15)
C6—C5—H5	120.4	C11—C12—H12	119.6
C5—C6—C1	121.82 (14)	C13—C12—H12	119.6
C5—C6—H6	119.1	C12—C13—C8	120.29 (14)
C1—C6—H6	119.1	C12—C13—H13	119.9
N1—C7—C1	111.91 (11)	C8—C13—H13	119.9
C6—C1—C2—O1	−178.32 (11)	C6—C1—C7—N1	−85.36 (15)
C7—C1—C2—O1	−0.22 (18)	C2—C1—C7—N1	96.59 (15)
C6—C1—C2—C3	−0.41 (19)	C7—N1—C8—C13	−166.89 (12)
C7—C1—C2—C3	177.69 (12)	C7—N1—C8—C9	16.20 (18)
O1—C2—C3—C4	178.62 (12)	C13—C8—C9—C10	−1.0 (2)

C1—C2—C3—C4	0.8 (2)	N1—C8—C9—C10	175.95 (13)
C2—C3—C4—C5	−0.5 (2)	C8—C9—C10—C11	0.3 (2)
C3—C4—C5—C6	−0.1 (2)	C9—C10—C11—C12	0.5 (3)
C4—C5—C6—C1	0.5 (2)	C10—C11—C12—C13	−0.7 (3)
C2—C1—C6—C5	−0.2 (2)	C11—C12—C13—C8	0.0 (3)
C7—C1—C6—C5	−178.35 (13)	C9—C8—C13—C12	0.8 (2)
C8—N1—C7—C1	177.20 (11)	N1—C8—C13—C12	−176.24 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	1.98	2.7871 (16)	170
N1—H1A···O1^{ii}	0.864 (16)	2.233 (16)	3.0770 (17)	165.8 (13)

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+2; (ii) *x*−1, *y*, *z*.

Fig. 1