Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-[(4-Methoxyanilino)methyl]phenol

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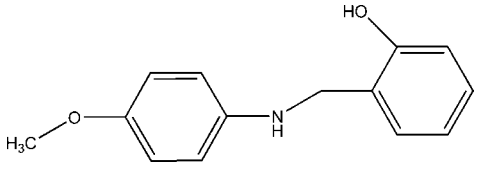
Received 2 August 2011; accepted 5 August 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.056; wR factor = 0.128; data-to-parameter ratio = 16.5.

In the title compound, $C_{14}H_{15}NO_2$, the dihedral angle between the two benzene rings is 71.10 (5)°. In the crystal, molecules are linked by intermolecular N—H···O, and O—H···N hydrogen bonds into a chain running parallel to the b axis.

Related literature

For the synthesis of the title compound, see: Noda (1959). For other related structures, see: Liu *et al.* (2007); Qu *et al.* (2007).



Experimental

Crystal data

$C_{14}H_{15}NO_2$
M_r = 229.27
Monoclinic, $P2_1/c$
a = 7.8132 (16) Å
b = 5.7947 (12) Å
c = 26.175 (5) Å
β = 95.02 (3)°
V = 1180.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.970, T_{max} = 0.983
10971 measured reflections
2693 independent reflections
1692 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.128
S = 1.03
2693 reflections
163 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86 (1)	2.22 (1)	3.058 (2)	163 (2)
O2—H2···N1^{ii}	0.86 (1)	1.89 (1)	2.741 (2)	172 (2)

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *SHELXL97*.

This work was supported by a start-up grant from Jiangsu University of Science and Technology and by the Foundation of Jiangsu Educational Committee (11KJB150004), China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2441).

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Noda, M. (1959). *J. Org. Chem.* **24**, 1209–1212.
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supplementary materials

Acta Cryst. (2011). E**67**, o2304 [**doi:10.1107/S1600536811031679**]

2-[(4-Methoxyanilino)methyl]phenol

H. Shu, N.-S. Yu, G.-L. Xie and L.-Z. Chen

Comment

Recently, the crystal structures of compounds closely related to the title molecule, *e.g.*, 2-[(4-chlorophenyl)aminomethyl]-6-methoxyphenol (Liu *et al.*, 2007) and 2-(anilinomethyl)phenol (Qu *et al.*, 2007) have been reported. We report here the crystal structure of a new member of this family of compounds.

In the title compound (Fig. 1), the dihedral angle between the two benzene ring planes is 71.10 (5)°. In the crystal structure, the molecules are linked by intermolecular N—H···O, and O—H···N hydrogen bonds into a one-dimensional chain lying parallel to the *b*-axis (Fig. 2).

Experimental

The title compound was synthesized by the reaction of 2-((4-methoxyphenylimino)- methyl)phenol (2.76 g, 10 mmol) with $NaBH_4$ (0.38 g, 10 mmol) in methanol (50 ml) according to the reported method (Noda, 1959). Crystals were obtained from an ethanolic (95%) solution by slow evaporation at room temperature.

Refinement

H atoms were placed at calculated positions and were included in the refinement in the riding-model approximation, with C—H = 0.93, 0.96 and 0.97 Å, for aryl, methyl and methylene H-atoms, respectively, with U_{iso}(H) = 1.2 (or 1.5 for methyl) U_{eq}(C). The hydrogen atoms bonded to O and N were included in the positions obtained from a difference map and were allowed to refine with distances contarined at N—H and O—H = 0.86 (1) Å.

Figures

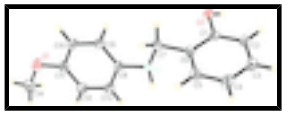

Fig. 1. The asymmetric unit of the title compound with atom labels. Displacement ellipsoids are drawn at the 30% probability level.

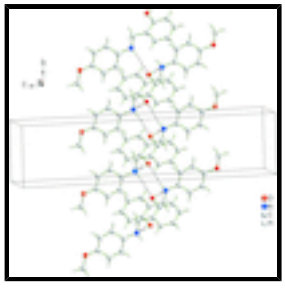

Fig. 2. The unit cell packing of the title compound viewed along the *b*-axis. Hydrogen bonds are drawn as dashed lines.

2-[(4-Methoxyanilino)methyl]phenol

Crystal data

$C_{14}H_{15}NO_2$	$F(000) = 488$
$M_r = 229.27$	$D_x = 1.290$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 8657 reflections
$a = 7.8132$ (16) Å	$\theta = 3.1$–$27.5°$
$b = 5.7947$ (12) Å	$\mu = 0.09$ mm^{-1}
$c = 26.175$ (5) Å	$T = 298$ K
$\beta = 95.02$ (3)°	Prism, colorless
$V = 1180.5$ (4) Å^3	0.40 × 0.30 × 0.20 mm
$Z = 4$	

Data collection

Rigaku SCXmini diffractometer	2693 independent reflections
Radiation source: fine-focus sealed tube	1692 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.056$
Detector resolution: 13.6612 pixels mm^{-1}	$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
CCD_Profile_fitting scans	$h = -9\rightarrow10$
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)	$k = -7\rightarrow7$
$T_{min} = 0.970$, $T_{max} = 0.983$	$l = -33\rightarrow33$
10971 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.056$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.128$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2 + 0.1931P]$ where $P = (F_o^2 + 2F_c^2)/3$
2693 reflections	$(\Delta/\sigma)_{max} < 0.001$
163 parameters	$\Delta\rho_{max} = 0.17$ e Å^{-3}
2 restraints	$\Delta\rho_{min} = -0.22$ e Å^{-3}

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.12511 (17)	0.7060 (2)	0.48819 (5)	0.0369 (4)
N1	0.1955 (2)	0.1501 (3)	0.54954 (6)	0.0322 (4)
C8	0.2161 (2)	0.0685 (3)	0.60126 (6)	0.0301 (4)
C7	0.3137 (2)	0.3330 (3)	0.53561 (7)	0.0350 (5)
H7A	0.4309	0.2888	0.5467	0.042*
H7B	0.2883	0.4746	0.5532	0.042*
C11	0.2449 (3)	−0.1048 (4)	0.70119 (7)	0.0395 (5)
C6	0.2976 (2)	0.3745 (3)	0.47851 (6)	0.0317 (4)
C1	0.2033 (2)	0.5582 (3)	0.45649 (6)	0.0295 (4)
C9	0.3148 (2)	0.1824 (3)	0.64015 (7)	0.0370 (5)
H9	0.3717	0.3180	0.6330	0.044*
O1	0.2685 (2)	−0.1765 (3)	0.75158 (5)	0.0600 (5)
C2	0.1942 (2)	0.5952 (3)	0.40425 (7)	0.0365 (5)
H2A	0.1322	0.7199	0.3900	0.044*
C10	0.3290 (3)	0.0950 (3)	0.68955 (7)	0.0410 (5)
H10	0.3961	0.1721	0.7152	0.049*
C13	0.1307 (3)	−0.1295 (3)	0.61362 (7)	0.0397 (5)
H13	0.0618	−0.2056	0.5882	0.048*
C5	0.3797 (3)	0.2304 (3)	0.44614 (8)	0.0442 (5)
H5	0.4435	0.1067	0.4601	0.053*
C12	0.1450 (3)	−0.2177 (4)	0.66294 (7)	0.0430 (5)
H12	0.0874	−0.3525	0.6703	0.052*
C4	0.3699 (3)	0.2647 (4)	0.39393 (8)	0.0488 (6)
H4	0.4257	0.1649	0.3731	0.059*
C3	0.2769 (3)	0.4478 (4)	0.37300 (7)	0.0437 (5)
H3	0.2696	0.4726	0.3378	0.052*
C14	0.1791 (4)	−0.3750 (4)	0.76569 (8)	0.0698 (8)
H14A	0.0576	−0.3478	0.7603	0.105*
H14B	0.2096	−0.4089	0.8012	0.105*
H14C	0.2092	−0.5034	0.7451	0.105*
H1	0.195 (2)	0.032 (2)	0.5294 (6)	0.046 (6)*
H2	0.0288 (19)	0.756 (4)	0.4738 (9)	0.083 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0365 (8)	0.0393 (8)	0.0342 (7)	0.0069 (7)	−0.0009 (6)	−0.0054 (6)

N1	0.0345 (9)	0.0315 (9)	0.0301 (9)	−0.0004 (7)	−0.0006 (7)	−0.0026 (7)
C8	0.0285 (10)	0.0322 (10)	0.0295 (9)	0.0057 (8)	0.0021 (8)	−0.0013 (8)
C7	0.0339 (11)	0.0342 (11)	0.0358 (10)	0.0013 (9)	−0.0029 (8)	0.0008 (8)
C11	0.0444 (12)	0.0466 (12)	0.0278 (10)	0.0049 (10)	0.0054 (9)	0.0003 (9)
C6	0.0299 (10)	0.0330 (10)	0.0319 (10)	−0.0002 (8)	0.0016 (8)	0.0000 (8)
C1	0.0267 (9)	0.0296 (10)	0.0325 (10)	−0.0044 (8)	0.0037 (8)	−0.0040 (8)
C9	0.0397 (11)	0.0355 (11)	0.0360 (11)	−0.0041 (9)	0.0036 (9)	−0.0029 (8)
O1	0.0814 (12)	0.0676 (11)	0.0304 (8)	−0.0100 (9)	0.0011 (8)	0.0072 (7)
C2	0.0355 (11)	0.0379 (11)	0.0355 (10)	0.0016 (9)	0.0005 (9)	0.0046 (9)
C10	0.0441 (12)	0.0468 (12)	0.0309 (10)	−0.0020 (10)	−0.0029 (9)	−0.0083 (9)
C13	0.0436 (12)	0.0420 (12)	0.0326 (10)	−0.0072 (9)	−0.0015 (9)	−0.0043 (9)
C5	0.0486 (13)	0.0406 (12)	0.0434 (12)	0.0136 (10)	0.0038 (10)	0.0013 (9)
C12	0.0496 (13)	0.0424 (12)	0.0372 (11)	−0.0101 (10)	0.0057 (10)	0.0023 (9)
C4	0.0520 (13)	0.0541 (14)	0.0415 (12)	0.0128 (11)	0.0106 (10)	−0.0083 (10)
C3	0.0455 (12)	0.0547 (13)	0.0317 (10)	−0.0011 (11)	0.0073 (9)	0.0000 (9)
C14	0.111 (2)	0.0580 (16)	0.0417 (13)	−0.0056 (15)	0.0122 (14)	0.0121 (11)

Geometric parameters (Å, °)

O2—C1	1.372 (2)	C9—H9	0.9300
O2—H2	0.862 (10)	O1—C14	1.412 (3)
N1—C8	1.430 (2)	C2—C3	1.382 (3)
N1—C7	1.472 (2)	C2—H2A	0.9300
N1—H1	0.864 (9)	C10—H10	0.9300
C8—C13	1.380 (3)	C13—C12	1.384 (3)
C8—C9	1.389 (2)	C13—H13	0.9300
C7—C6	1.508 (2)	C5—C4	1.376 (3)
C7—H7A	0.9700	C5—H5	0.9300
C7—H7B	0.9700	C12—H12	0.9300
C11—C10	1.378 (3)	C4—C3	1.372 (3)
C11—C12	1.379 (3)	C4—H4	0.9300
C11—O1	1.380 (2)	C3—H3	0.9300
C6—C5	1.386 (3)	C14—H14A	0.9600
C6—C1	1.390 (2)	C14—H14B	0.9600
C1—C2	1.380 (2)	C14—H14C	0.9600
C9—C10	1.384 (3)		
C1—O2—H2	111.4 (17)	C1—C2—H2A	119.8
C8—N1—C7	116.84 (14)	C3—C2—H2A	119.8
C8—N1—H1	108.1 (13)	C11—C10—C9	120.88 (18)
C7—N1—H1	112.8 (13)	C11—C10—H10	119.6
C13—C8—C9	118.17 (17)	C9—C10—H10	119.6
C13—C8—N1	118.71 (16)	C8—C13—C12	121.63 (18)
C9—C8—N1	123.10 (17)	C8—C13—H13	119.2
N1—C7—C6	111.14 (15)	C12—C13—H13	119.2
N1—C7—H7A	109.4	C4—C5—C6	122.09 (19)
C6—C7—H7A	109.4	C4—C5—H5	119.0
N1—C7—H7B	109.4	C6—C5—H5	119.0
C6—C7—H7B	109.4	C11—C12—C13	119.77 (19)
H7A—C7—H7B	108.0	C11—C12—H12	120.1

C10—C11—C12	119.22 (18)	C13—C12—H12	120.1
C10—C11—O1	115.96 (18)	C3—C4—C5	119.31 (19)
C12—C11—O1	124.81 (19)	C3—C4—H4	120.3
C5—C6—C1	117.69 (17)	C5—C4—H4	120.3
C5—C6—C7	120.43 (17)	C4—C3—C2	120.01 (18)
C1—C6—C7	121.88 (16)	C4—C3—H3	120.0
O2—C1—C2	121.01 (16)	C2—C3—H3	120.0
O2—C1—C6	118.35 (15)	O1—C14—H14A	109.5
C2—C1—C6	120.59 (16)	O1—C14—H14B	109.5
C10—C9—C8	120.31 (18)	H14A—C14—H14B	109.5
C10—C9—H9	119.8	O1—C14—H14C	109.5
C8—C9—H9	119.8	H14A—C14—H14C	109.5
C11—O1—C14	117.88 (17)	H14B—C14—H14C	109.5
C1—C2—C3	120.31 (18)		
C7—N1—C8—C13	−168.27 (16)	C6—C1—C2—C3	0.9 (3)
C7—N1—C8—C9	13.4 (2)	C12—C11—C10—C9	−0.3 (3)
C8—N1—C7—C6	170.60 (14)	O1—C11—C10—C9	179.82 (18)
N1—C7—C6—C5	−80.6 (2)	C8—C9—C10—C11	−0.5 (3)
N1—C7—C6—C1	100.3 (2)	C9—C8—C13—C12	−1.6 (3)
C5—C6—C1—O2	−178.27 (16)	N1—C8—C13—C12	−179.97 (17)
C7—C6—C1—O2	0.8 (3)	C1—C6—C5—C4	−0.1 (3)
C5—C6—C1—C2	−0.6 (3)	C7—C6—C5—C4	−179.12 (19)
C7—C6—C1—C2	178.44 (17)	C10—C11—C12—C13	0.1 (3)
C13—C8—C9—C10	1.3 (3)	O1—C11—C12—C13	179.99 (18)
N1—C8—C9—C10	179.69 (17)	C8—C13—C12—C11	0.8 (3)
C10—C11—O1—C14	177.40 (19)	C6—C5—C4—C3	0.4 (3)
C12—C11—O1—C14	−2.5 (3)	C5—C4—C3—C2	−0.1 (3)
O2—C1—C2—C3	178.53 (17)	C1—C2—C3—C4	−0.6 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86 (1)	2.22 (1)	3.058 (2)	163 (2)
O2—H2···N1^{ii}	0.86 (1)	1.89 (1)	2.741 (2)	172 (2)

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

Fig. 1

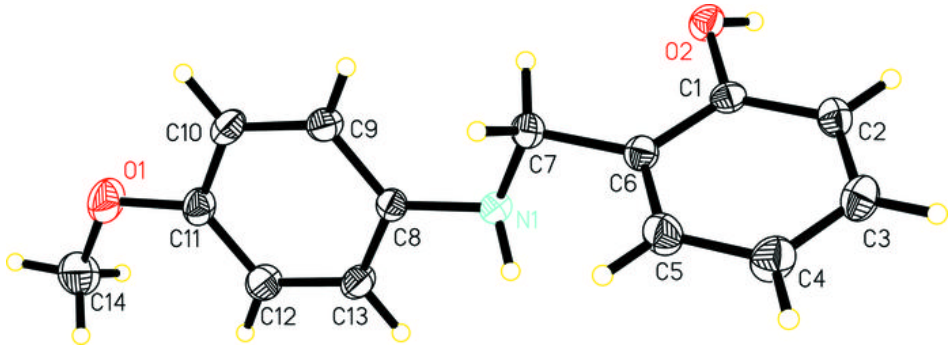

Fig. 2