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## Key indicators

Single-crystal X-ray study  
 $T = 296$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.050  
 $wR$  factor = 0.149  
Data-to-parameter ratio = 15.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## 4-(Hexyloxy)aniline

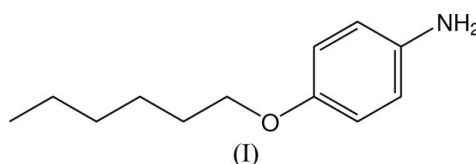
The title molecule,  $\text{C}_{12}\text{H}_{19}\text{NO}$ , crystallizes with a head-to-head tail-to-tail arrangement, including very weak  $\text{N}-\text{H} \cdots \text{N}$  and  $\text{N}-\text{H} \cdots \text{O}$  hydrogen bonds.

Received 5 September 2005

Accepted 6 September 2005

Online 14 September 2005

## Comment

Low molecular weight imines (Demus *et al.*, 1998; Sudhakar *et al.*, 2000) and polyimines (Natansohn *et al.*, 1991) with mesomorphic behavior continue to be studied. The title compound, (I), is the starting material for the synthesis of some imines by condensation with functionalized aldehydes. A suitable functionalization of these imines with allyl groups may afford polymerizable monomers (López *et al.*, 2005).

Compound (I) is stabilized in the solid state as a bent molecule (Fig. 1) due to the *gauche* conformation of the alkyl chain with respect to the aryl moiety [ $\text{O1}-\text{C7}-\text{C8}-\text{C9} = 70.1$  ( $3^\circ$ )]. Geometric parameters (Table 1) are as expected. For instance, the amine group presents a pyramidal arrangement of bonds around the N atom, very close to that observed for aniline. One measure of the *s* or *p* character of the N atoms in primary amines is given by the angle between the C—N bond and the bisector of the H—N—H angle (Carey, 2003). In the case of aniline, for which the structure has been determined at 252 K (Fukuyo *et al.*, 1982), this angle is 139.1 and 141.1° for two independent molecules, while for (I), the equivalent angle is 140.6 ( $4^\circ$ ). It is thus clear that the *para* substitution of the aniline by a hexyloxy group has very little influence on the amine functionality.

A common head-to-head tail-to-tail arrangement is observed for the crystal structure (Fig. 2). The angle between

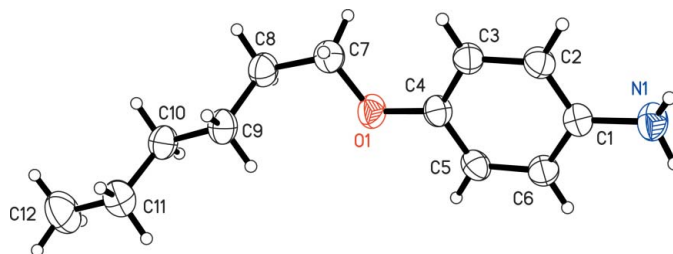


Figure 1

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

two neighboring benzene rings is  $76.62(6)^\circ$  (rings related by symmetry code  $\frac{1}{2} + x, y, \frac{3}{2} - z$ ). As the O atom of an alkoxy group is a very poor donor and acceptor for hydrogen bonding, very weak intermolecular interactions are observed in the crystal structure (Table 2); N—H $\cdots$ N bonds link molecules along [100] and N—H $\cdots$ O interactions link molecules along [010]. The weakness of these intermolecular contacts, together with the low molecular weight of (I), may be related to the low melting point for this material (m.p. 316 K).

## Experimental

Compound (I) was prepared by reacting 4-hydroxyphenylacetamide and 1-bromohexane, as described in the literature (Sudhakar *et al.*, 2000), and was crystallized from hexane as dark brown crystals. Analysis found: C 74.6, H 9.8, O 8.3, N 7.2%; calculated for  $C_{12}H_{19}NO$ : C 74.6, H 9.8, O 8.2, N 7.2%.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  0.89 (*d*,  $J = 6.4$  Hz, 3H,  $CH_3$ ), 1.32–1.42 (*m*,  $J = 6.8, 5.6$  Hz, 6H,  $3 \times CH_2$ ), 1.73 (*m*,  $J = 6.8, 7.2$  Hz, 2H,  $CH_2$ ), 3.21 (*s*, 2H,  $NH_2$ ), 3.87 (*m*,  $J = 6.8, 6.4$  Hz, 2H, O— $CH_2$ ), 6.25 (*m*,  $J = 8.8$  Hz, 2H, Ph), 6.74 (*m*,  $J = 8.8$  Hz, 2H, Ph).

### Crystal data

$C_{12}H_{19}NO$	Mo $K\alpha$ radiation
$M_r = 193.28$	Cell parameters from 75 reflections
Orthorhombic, <i>Pbca</i>	$\theta = 4.8$ – $12.5^\circ$
$a = 5.4659(10)$ Å	$\mu = 0.07$ mm $^{-1}$
$b = 13.6278(19)$ Å	$T = 296(2)$ K
$c = 32.124(4)$ Å	Irregular fragment, colorless
$V = 2392.8(6)$ Å $^3$	$0.6 \times 0.3 \times 0.3$ mm
$Z = 8$	
$D_x = 1.073$ Mg m $^{-3}$	

### Data collection

Bruker P4 diffractometer	$\theta_{max} = 25.0^\circ$
$2\theta/\omega$ scans	$h = -6 \rightarrow 2$
Absorption correction: none	$k = -16 \rightarrow 1$
3385 measured reflections	$l = -38 \rightarrow 1$
2111 independent reflections	2 standard reflections
1159 reflections with $I > 2\sigma(I)$	every 48 reflections
$R_{int} = 0.031$	intensity decay: 2.5%

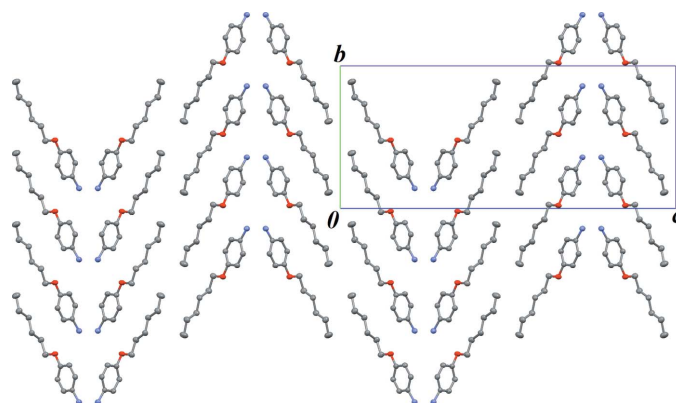
### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 0.637P]$
$R[F^2 > 2\sigma(F^2)] = 0.050$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.149$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.13$ e Å $^{-3}$
2111 reflections	$\Delta\rho_{min} = -0.18$ e Å $^{-3}$
137 parameters	Extinction correction:
H atoms treated by a mixture of independent and constrained refinement	<i>SHELXTL-Plus</i>
	Extinction coefficient: 0.0112 (16)

**Table 1**

Selected geometric parameters (Å, °).

O1—C4	1.384 (3)	C7—C8	1.512 (3)
O1—C7	1.427 (3)	C8—C9	1.510 (3)
N1—C1	1.407 (3)	C9—C10	1.519 (3)
N1—H1A	0.90 (3)	C10—C11	1.502 (3)
N1—H1B	0.87 (3)	C11—C12	1.521 (4)
C4—O1—C7	118.22 (18)	C1—N1—H1B	112.8 (18)
C1—N1—H1A	117.2 (18)	H1A—N1—H1B	114 (3)



**Figure 2**

Part of the crystal structure of (I), viewed along the [100] axis. H atoms have been omitted.

**Table 2**

Hydrogen-bond geometry (Å, °).

D—H $\cdots$ A	D—H	H $\cdots$ A	D $\cdots$ A	D—H $\cdots$ A
N1—H1A $\cdots$ N1 <sup>i</sup>	0.90 (3)	2.40 (3)	3.277 (3)	166 (2)
N1—H1B $\cdots$ O1 <sup>ii</sup>	0.87 (3)	2.38 (3)	3.217 (3)	162 (2)

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

The H atoms bonded to N1 were found in a difference map and refined with free coordinates and isotropic  $U$  parameters. H atoms bonded to C atoms were placed in idealized positions and refined as riding on their parent C atom [C—H distances and isotropic  $U_{iso}(H)$  parameters: methylene 0.97 Å and  $1.2U_{eq}(C)$ ; methyl 0.96 Å and  $1.5U_{eq}(C)$ ; aromatic 0.93 Å and  $1.2U_{eq}(C)$ ].

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *SHELXTL-Plus*; software used to prepare material for publication: *SHELXTL-Plus*.

Partial support by VIEP–BUAP/CONACyT (project No. 7/I/NAT/05) is gratefully acknowledged. AMH is indebted to PROMEP (Mexico) for providing a research grant.

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