(E)-2-Methyl-4-[(4-propylphenyl)-diazenyl]phenol

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The title compound, $C_{16}H_{18}N_2O$, was produced when 4-propylbenzenediazonium chloride, prepared from a 4-propylaniline and $NaNO_2$–HCl mixture, was treated with 2-methylphenol in an approximately 1:1 molar ratio. The molecules of the title compound are stabilized by inversion-related O—H···N and C—H···O intermolecular hydrogen bonds. The O—H···N and C—H···O hydrogen bonds generate two edge-fused $R_2^2(6)$ ring motifs. The dihedral angle between the aromatic rings is 15.28 (10)°. The N atoms are disordered approximately equally over two positions.

Related literature

For related literature, see: Albayrak *et al.* (2004, 2007); Etter (1990); Garg & Sharma (1969); Odabaşoğlu *et al.* (2003); Peters & Freeman (1991); Ravindranath *et al.* (1983); Şahin *et al.* (2005a,b,c,d,e).
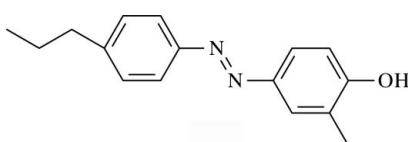
Experimental

Crystal data

$C_{16}H_{18}N_2O$	$V = 2866.0$ (4) Å^3
$M_r = 254.32$	$Z = 8$
Orthorhombic, $Pbca$	Mo $K\alpha$ radiation
$a = 9.9032$ (7) Å	$\mu = 0.08$ mm^{-1}
$b = 12.0663$ (8) Å	$T = 296$ K
$c = 23.984$ (2) Å	$0.72 \times 0.51 \times 0.19$ mm

Data collection

Stoe IPDS2 diffractometer	30080 measured reflections
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)	2813 independent reflections
	1315 reflections with $I > 2\sigma(I)$
$T_{min} = 0.958$, $T_{max} = 0.986$	$R_{int} = 0.129$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.177$	
$S = 0.91$	
2813 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
176 parameters	$\Delta\rho_{min} = -0.15$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2A^i	0.95 (4)	1.94 (4)	2.877 (4)	170 (3)
O1—H1···N1B^i	0.95 (4)	2.03 (4)	2.964 (5)	169 (3)
C6—H6···O1^{ii}	0.93	2.63	3.454 (3)	147
C9—H9···O1^{ii}	0.93	2.77	3.443 (4)	131

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (ii) $x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); 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: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2363).

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supplementary materials

(*E*)-2-Methyl-4-[(4-propylphenyl)diazenyl]phenol

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Comment

Azobenzene derivatives have been the most widely used class of dyes due to their versatile application in various fields, such as dyeing textile fibers, biomedical studies, advanced applications in organic synthesis, and high technology areas as laser, liquid crystalline displays, electro-optical devices, and ink-jet printers (Peters & Freeman, 1991). In the azo class of dye molecules, azo compounds are an important type of organic colorants and consist of at least a conjugated chromophore azo group and two or more aromatic rings. The colour of an azo dye is mainly due to the interaction of the azo group with incident light. The pharmaceutical importance of compounds including an arylazo group has been extensively reported in the literature (Garg & Sharma, 1969). The oxidation-reduction behaviors of these compounds play an important role in its biological activity (Ravindranath *et al.*, 1983). In view of the importance of the title compound, (I), a crystal structure is investigated. The present work is part of a structural study of compounds of phenolicazobenzene (Albayrak *et al.*, 2007, 2004; Odabaşoğlu *et al.*, 2003; Şahin *et al.*, 2005*a*,b,c,d,e) and we report here the structure of the title compound (Fig. 1).

The molecular structure of (I) is shown in Fig. 1, with the atom-numbering scheme. Selected bond distances and angles are given in Table 1. The a rings aromatic adopt a *trans* configuration about the azo functional group and dihedral angle between the rings is 15.28 (10)°. All the C—C bond lengths in the C1—C6 and C8—C13 rings have typical C_{sp2}—C_{sp2} values. The average C—C bond lengths within these two rings are 1.380 (4) and 1.369 (4) A °, respectively. In the azo group, the C—N and N=N bond lenghths different normal C—N and N=N bonds and angles of around the N atoms are abnormal because of orientational disorder (Fig. 1). The title molecules are stabilized by O—H···N and C—H···O intermolecular hydrogen bonds and O—H···N and C—H···O hydrogen bonds generate hydrogen bonded chain which have edge-fussed $[R_2^2(6)R_2^2(6)]$ ring motifs (Fig. 2, Table 2) (Etter, 1990). The hydrogen bonded chains arranged as forming quardrangle tunnels (Fig. 3).

Experimental

A mixture of 4-propylaniline (1.352 g, 10 mmol), water (50 ml) and concentrated hydrochloric acid (2.5 ml, 30 mmol) was heated with stirring until a clear solution was obtained. This solution was cooled down to 273–278 K and a solution of sodium nitrite (0.96 g, 14 mmol) in water was added dropwise while the temperature was maintained below 278 K. The resulting mixture was stirred for 30 min in an ice bath. 2-methylphenol (1.081 g, 10 mmol) solution (pH 9) was gradually added to a cooled solution of 4-propylbenzenediazonium chloride, prepared as described above, and the resulting mixture was stirred at 273–278 K for 60 min in an ice bath. The product was recrystallized from acetonitrile to obtain solid (*E*)-2-methyl-4-[(4-propylphenyl) diazenyl]phenol (Yield 31%; m.p. 384–386 K).

Refinement

All C-bound H atoms were refined using the riding model approximation with d(C—H) = 0.93 for aromatic, d(C—H) = 0.97 for methylene and d(C—H) = 0.96 for methyl C—H [U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C)]. O-bound H atom was located in Fourier difference map and refined freely due to its taking part in H-bond. The two N atoms in the azo

supplementary materials

group are orientational disorder. The relative occupancies for the disordered components were refined freely to yield relative occupancies of 0.501 (8) and 0.499 (8), respectively, for N1A (N1B) and N2A (N2B).

Figures
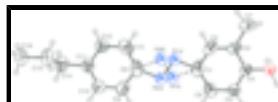
Fig. 1. A view of (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level..
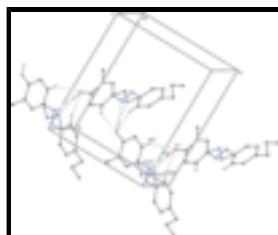

Fig. 2. Part of the crystal structure of (I), showing the formation of $R_2^2(6)R_2^2(6)$ motifs. [Symmetry code: (i) $-x$, $3/2 - y$, $1 - z$].
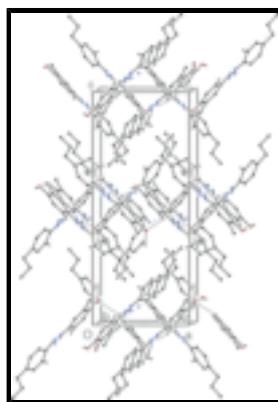
Fig. 3. A packing diagram of (I), showing the quardrangle tunnels. H atoms not involved in intramolecular interactions have been ommited for clarity.

(E)-2-Methyl-4-[(4-propylphenyl)diazenyl]phenol

Crystal data

$C_{16}H_{18}N_2O$	$F_{000} = 1088$
$M_r = 254.32$	$D_x = 1.179$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ac 2ab	Cell parameters from 22722 reflections
$a = 9.9032$ (7) Å	$\theta = 1.7–26.0°$
$b = 12.0663$ (8) Å	$\mu = 0.08$ mm^{-1}
$c = 23.984$ (2) Å	$T = 296$ K
$V = 2866.0$ (4) Å^3	Prism, brown
$Z = 8$	$0.72 \times 0.51 \times 0.19$ mm

Data collection

Stoe IPDS2 diffractometer	2813 independent reflections
Monochromator: plane graphite	1315 reflections with $I > 2\sigma(I)$

Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.129$
$T = 296$ K	$\theta_{max} = 26.0°$
ω scan rotation method	$\theta_{min} = 1.7°$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$h = -12 \rightarrow 12$
$T_{min} = 0.958$, $T_{max} = 0.986$	$k = -14 \rightarrow 14$
30080 measured reflections	$l = -29 \rightarrow 29$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.0964P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.177$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.91$	$\Delta\rho_{max} = 0.19$ e Å^{-3}
2813 reflections	$\Delta\rho_{min} = -0.15$ e Å^{-3}
176 parameters	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0041 (13)
Secondary atom site location: difference Fourier map	

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	$U_{iso}*/U_{eq}$	Occ. (<1)
C1	0.2475 (3)	0.5850 (3)	0.51406 (13)	0.1011 (9)	
C2	0.1876 (3)	0.5164 (2)	0.47522 (13)	0.0972 (9)	
H2	0.2122	0.4420	0.4746	0.117*	
C3	0.0941 (3)	0.55263 (18)	0.43763 (11)	0.0814 (7)	
C4	0.0579 (2)	0.66430 (19)	0.43955 (10)	0.0721 (6)	
C5	0.1156 (3)	0.7349 (2)	0.47817 (10)	0.0815 (7)	
H5	0.0906	0.8092	0.4791	0.098*	
C6	0.2098 (3)	0.6956 (3)	0.51507 (11)	0.0952 (8)	

H6	0.2486	0.7434	0.5409	0.114*	
C7	0.0314 (3)	0.4775 (2)	0.39447 (13)	0.1125 (10)	
H7A	0.0512	0.5053	0.3579	0.135*	
H7B	−0.0646	0.4753	0.3998	0.135*	
H7C	0.0678	0.4042	0.3983	0.135*	
C8	0.4872 (3)	0.4888 (4)	0.61056 (13)	0.1068 (10)	
C9	0.5234 (4)	0.5440 (3)	0.65733 (15)	0.1279 (11)	
H9	0.4860	0.6132	0.6647	0.153*	
C10	0.6148 (4)	0.4991 (3)	0.69411 (13)	0.1197 (10)	
H10	0.6376	0.5387	0.7260	0.144*	
C11	0.6733 (3)	0.3979 (2)	0.68518 (11)	0.0897 (7)	
C12	0.6357 (3)	0.3422 (2)	0.63816 (12)	0.0965 (8)	
H12	0.6731	0.2730	0.6309	0.116*	
C13	0.5443 (3)	0.3858 (3)	0.60142 (12)	0.1081 (10)	
H13	0.5203	0.3456	0.5699	0.130*	
C14	0.7710 (3)	0.3489 (3)	0.72635 (14)	0.1183 (10)	
H14A	0.8407	0.3098	0.7059	0.142*	
H14B	0.8143	0.4090	0.7464	0.142*	
C15	0.7113 (3)	0.2718 (3)	0.76744 (13)	0.1191 (11)	
H15A	0.6711	0.2102	0.7475	0.143*	
H15B	0.6393	0.3100	0.7870	0.143*	
C16	0.8075 (3)	0.2271 (3)	0.80925 (12)	0.1238 (11)	
H16A	0.8469	0.2872	0.8298	0.149*	
H16B	0.8774	0.1864	0.7906	0.149*	
H16C	0.7603	0.1788	0.8344	0.149*	
N1A	0.3301 (5)	0.5099 (4)	0.54315 (18)	0.0729 (15)*	0.501 (8)
N2A	0.3998 (5)	0.5696 (4)	0.5811 (2)	0.0699 (14)*	0.499 (8)
N1B	0.3534 (6)	0.5833 (4)	0.5619 (2)	0.0784 (15)*	0.501 (8)
N2B	0.3897 (6)	0.4875 (4)	0.5616 (2)	0.0814 (16)*	0.499 (8)
O1	−0.03469 (18)	0.70055 (15)	0.40199 (7)	0.0866 (5)	
H1	−0.066 (3)	0.774 (3)	0.4090 (13)	0.134 (12)*	

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0825 (17)	0.130 (3)	0.0903 (19)	0.0218 (17)	0.0118 (15)	0.0385 (19)
C2	0.0960 (19)	0.0829 (18)	0.113 (2)	0.0185 (15)	0.0253 (18)	0.0296 (17)
C3	0.0844 (16)	0.0634 (14)	0.0964 (18)	−0.0017 (12)	0.0231 (14)	0.0035 (13)
C4	0.0757 (14)	0.0680 (13)	0.0726 (14)	0.0016 (11)	0.0078 (12)	0.0051 (12)
C5	0.0899 (16)	0.0750 (14)	0.0795 (15)	0.0021 (13)	0.0030 (14)	−0.0058 (13)
C6	0.0883 (18)	0.123 (2)	0.0737 (16)	−0.0010 (17)	0.0014 (14)	−0.0001 (15)
C7	0.126 (2)	0.0725 (17)	0.139 (3)	−0.0154 (16)	0.028 (2)	−0.0195 (17)
C8	0.0867 (19)	0.148 (3)	0.086 (2)	0.0006 (19)	0.0052 (15)	0.031 (2)
C9	0.155 (3)	0.115 (2)	0.114 (2)	0.040 (2)	−0.010 (2)	0.012 (2)
C10	0.159 (3)	0.098 (2)	0.102 (2)	0.011 (2)	−0.028 (2)	−0.0089 (18)
C11	0.0880 (17)	0.0883 (18)	0.0927 (18)	−0.0064 (14)	−0.0056 (15)	0.0112 (15)
C12	0.109 (2)	0.0877 (17)	0.0931 (19)	−0.0100 (15)	0.0084 (17)	0.0004 (16)
C13	0.107 (2)	0.142 (3)	0.0756 (18)	−0.040 (2)	0.0029 (17)	0.0059 (19)

C14	0.097 (2)	0.129 (2)	0.129 (2)	−0.0041 (18)	−0.0163 (19)	0.019 (2)
C15	0.096 (2)	0.161 (3)	0.101 (2)	0.0069 (19)	−0.0072 (17)	0.033 (2)
C16	0.114 (2)	0.156 (3)	0.102 (2)	0.009 (2)	−0.0160 (18)	0.016 (2)
O1	0.0941 (12)	0.0756 (11)	0.0902 (12)	0.0075 (9)	−0.0089 (10)	−0.0095 (9)

Geometric parameters (Å, °)

C1—C2	1.380 (4)	C9—H9	0.9300
C1—C6	1.386 (4)	C10—C11	1.368 (4)
C1—N1A	1.406 (6)	C10—H10	0.9300
C1—N1B	1.554 (8)	C11—C12	1.364 (4)
C2—C3	1.365 (4)	C11—C14	1.504 (4)
C2—H2	0.9300	C12—C13	1.368 (4)
C3—C4	1.395 (3)	C12—H12	0.9300
C3—C7	1.509 (4)	C13—H13	0.9300
C4—O1	1.358 (3)	C14—C15	1.478 (4)
C4—C5	1.383 (3)	C14—H14A	0.9700
C5—C6	1.370 (3)	C14—H14B	0.9700
C5—H5	0.9300	C15—C16	1.485 (4)
C6—H6	0.9300	C15—H15A	0.9700
C7—H7A	0.9600	C15—H15B	0.9700
C7—H7B	0.9600	C16—H16A	0.9600
C7—H7C	0.9600	C16—H16B	0.9600
C8—C9	1.353 (5)	C16—H16C	0.9600
C8—C13	1.383 (5)	N1A—N2A	1.350 (6)
C8—N2A	1.483 (7)	N1B—N2B	1.211 (6)
C8—N2B	1.521 (7)	O1—H1	0.95 (4)
C9—C10	1.376 (4)		
C2—C1—C6	118.3 (3)	C11—C10—H10	119.0
C2—C1—N1A	101.4 (3)	C9—C10—H10	119.0
C6—C1—N1A	140.2 (4)	C12—C11—C10	117.0 (3)
C2—C1—N1B	141.3 (3)	C12—C11—C14	121.6 (3)
C6—C1—N1B	100.5 (3)	C10—C11—C14	121.4 (3)
C3—C2—C1	123.1 (3)	C11—C12—C13	121.6 (3)
C3—C2—H2	118.5	C11—C12—H12	119.2
C1—C2—H2	118.5	C13—C12—H12	119.2
C2—C3—C4	117.5 (2)	C12—C13—C8	120.9 (3)
C2—C3—C7	122.7 (3)	C12—C13—H13	119.5
C4—C3—C7	119.8 (3)	C8—C13—H13	119.5
O1—C4—C5	121.7 (2)	C15—C14—C11	115.3 (2)
O1—C4—C3	117.6 (2)	C15—C14—H14A	108.4
C5—C4—C3	120.7 (2)	C11—C14—H14A	108.4
C6—C5—C4	120.1 (2)	C15—C14—H14B	108.4
C6—C5—H5	120.0	C11—C14—H14B	108.4
C4—C5—H5	120.0	H14A—C14—H14B	107.5
C5—C6—C1	120.4 (3)	C14—C15—C16	115.0 (3)
C5—C6—H6	119.8	C14—C15—H15A	108.5
C1—C6—H6	119.8	C16—C15—H15A	108.5
C3—C7—H7A	109.5	C14—C15—H15B	108.5

C3—C7—H7B	109.5	C16—C15—H15B	108.5
H7A—C7—H7B	109.5	H15A—C15—H15B	107.5
C3—C7—H7C	109.5	C15—C16—H16A	109.5
H7A—C7—H7C	109.5	C15—C16—H16B	109.5
H7B—C7—H7C	109.5	H16A—C16—H16B	109.5
C9—C8—C13	117.8 (3)	C15—C16—H16C	109.5
C9—C8—N2A	103.0 (4)	H16A—C16—H16C	109.5
C13—C8—N2A	138.9 (4)	H16B—C16—H16C	109.5
C9—C8—N2B	144.4 (4)	N2A—N1A—C1	106.7 (4)
C13—C8—N2B	97.3 (3)	N1A—N2A—C8	105.6 (4)
C8—C9—C10	120.8 (3)	N2B—N1B—C1	102.0 (5)
C8—C9—H9	119.6	N1B—N2B—C8	100.0 (5)
C10—C9—H9	119.6	C4—O1—H1	114 (2)
C11—C10—C9	122.0 (3)		
C6—C1—C2—C3	0.5 (4)	C14—C11—C12—C13	178.4 (3)
N1A—C1—C2—C3	178.2 (2)	C11—C12—C13—C8	0.5 (4)
N1B—C1—C2—C3	−179.0 (3)	C9—C8—C13—C12	−0.9 (5)
C1—C2—C3—C4	−0.5 (4)	N2A—C8—C13—C12	172.1 (4)
C1—C2—C3—C7	178.6 (2)	N2B—C8—C13—C12	−175.1 (3)
C2—C3—C4—O1	179.7 (2)	C12—C11—C14—C15	−83.1 (4)
C7—C3—C4—O1	0.5 (3)	C10—C11—C14—C15	94.8 (4)
C2—C3—C4—C5	0.2 (3)	C11—C14—C15—C16	−177.8 (3)
C7—C3—C4—C5	−179.0 (2)	C2—C1—N1A—N2A	177.0 (3)
O1—C4—C5—C6	−179.3 (2)	C6—C1—N1A—N2A	−6.2 (6)
C3—C4—C5—C6	0.2 (3)	N1B—C1—N1A—N2A	−0.3 (3)
C4—C5—C6—C1	−0.2 (4)	C1—N1A—N2A—C8	−179.3 (3)
C2—C1—C6—C5	−0.1 (4)	C9—C8—N2A—N1A	−162.7 (3)
N1A—C1—C6—C5	−176.5 (3)	C13—C8—N2A—N1A	23.7 (6)
N1B—C1—C6—C5	179.6 (2)	N2B—C8—N2A—N1A	4.9 (3)
C13—C8—C9—C10	0.5 (5)	C2—C1—N1B—N2B	0.5 (6)
N2A—C8—C9—C10	−174.8 (3)	C6—C1—N1B—N2B	−179.2 (3)
N2B—C8—C9—C10	170.7 (4)	N1A—C1—N1B—N2B	4.7 (3)
C8—C9—C10—C11	0.3 (6)	C1—N1B—N2B—C8	−177.3 (2)
C9—C10—C11—C12	−0.7 (5)	C9—C8—N2B—N1B	19.9 (7)
C9—C10—C11—C14	−178.8 (3)	C13—C8—N2B—N1B	−168.9 (3)
C10—C11—C12—C13	0.4 (4)	N2A—C8—N2B—N1B	−1.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2A[i]	0.95 (4)	1.94 (4)	2.877 (4)	170 (3)
O1—H1···N1B[i]	0.95 (4)	2.03 (4)	2.964 (5)	169 (3)
C6—H6···O1[ii]	0.93	2.63	3.454 (3)	147
C9—H9···O1[ii]	0.93	2.77	3.443 (4)	131

Symmetry codes: (i) *x*−1/2, −*y*+3/2, −*z*+1; (ii) *x*+1/2, −*y*+3/2, −*z*+1.

Fig. 1

Fig. 2

Fig. 3