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3-{[(2,6-Diisopropylphenyl)imino]methyl}-2-naphthol

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In the title molecule, $C_{23}H_{25}NO$, the hydroxy H atom is involved in the formation of an intramolecular O—H···N hydrogen bond. The dihedral angle between the benzene ring and the 2-naphthol system is 78.1 (1)°. The crystal packing is stabilized by van der Waals forces.

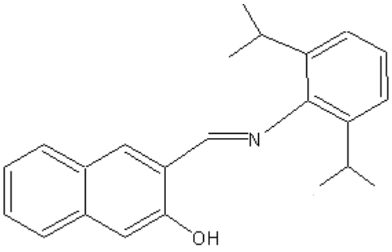
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.054
wR factor = 0.166
Data-to-parameter ratio = 16.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

A number of 2-hydroxy-substituted Schiff base ligands derived from the reaction of 2-hydroxy-1-naphthaldehyde with amines have been structurally characterized because of their ability to bind transition metal ions; these include 3-{[(2-ethanol)imino]methyl}-2-naphthol (Kaitner & Pavlović, 1999), 3-{[(2-pyridyl)imino]methyl}-2-naphthol, 3-{[(1,1-dimethy-2-ethanol)imino]methyl}-2-naphthol and two similar compounds (Rao *et al.*, 2003). As part of a study of the coordination chemistry of such ligands, we report here the crystal structure of the title compound, (I) (Fig. 1).



(I)

Selected bond lengths and angles of (I) are listed in Table 1. The conformation of (I) is characterized by the C12—N1—C11—C10 torsion angle of 176.27 (18)° and the dihedral angle between the benzene ring and 2-naphthol group of 78.1 (1)°. Hydroxy atom H1 is involved in the formation of an intramolecular O—H···N hydrogen bond (Table 2). The crystal packing is stabilized by van der Waals forces.

Experimental

The title compound was synthesized by refluxing methanol solutions (25 ml) of 2-hydroxy-1-naphthaldehyde (1.72 g, 10 mmol) and 2,6-diisopropylaniline (10 mmol), using triethylamine as catalytic agent. The yellow crystalline product was obtained from the deep yellow coloured solution after it had been left to stand for a few days. The precipitate was filtered off and washed with cold methanol (yield 49%); single crystals of good diffraction quality were obtained by evaporation of its chloroform solution. Analysis calculated for $C_{23}H_{25}NO$: C 83.34, H 7.60, N 4.23%; found: C 83.41, H 7.57, N 4.27%.

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Crystal data

$C_{23}H_{25}NO$
$M_r = 331.44$
Monoclinic, $P2_1/n$
$a = 9.3365\ (11)$ Å
$b = 22.824\ (5)$ Å
$c = 9.3508\ (12)$ Å
$\beta = 98.629\ (8)^\circ$
$V = 1970.0\ (6)$ Å^3
$Z = 4$
$D_x = 1.117$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 831 reflections
$\theta = 2.4$–23.6°
$\mu = 0.07$ mm^{-1}
$T = 293\ (2)$ K
Prism, yellow
0.38 × 0.36 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.794$, $T_{\max} = 0.980$
11 528 measured reflections
4091 independent reflections
2096 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.039$
$\theta_{\max} = 26.5^\circ$
$h = -11 \rightarrow 11$
$k = -20 \rightarrow 28$
$l = -8 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.166$
$S = 1.01$
4091 reflections
254 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0715P)^2 + 0.2668P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.24$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}
Extinction correction: none

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.334 (3)	C2—C3	1.343 (3)
O1—H1	0.846 (10)	C3—C4	1.416 (3)
N1—C11	1.285 (2)	C9—C10	1.435 (3)
N1—C12	1.426 (2)	C10—C11	1.438 (2)
C1—C10	1.394 (3)	C12—C13	1.393 (3)
C1—C2	1.406 (3)		
C1—O1—H1	107 (2)	C8—C9—C10	123.73 (18)
C11—N1—C12	122.58 (17)	C4—C9—C10	119.27 (19)
O1—C1—C10	122.40 (18)	C1—C10—C9	119.20 (17)
O1—C1—C2	117.0 (2)	C1—C10—C11	118.96 (17)
C10—C1—C2	120.6 (2)	C9—C10—C11	121.84 (18)
C3—C2—C1	120.0 (2)	N1—C11—C10	121.27 (19)
C8—C9—C4	117.00 (19)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.846 (10)	1.727 (18)	2.501 (2)	151 (3)

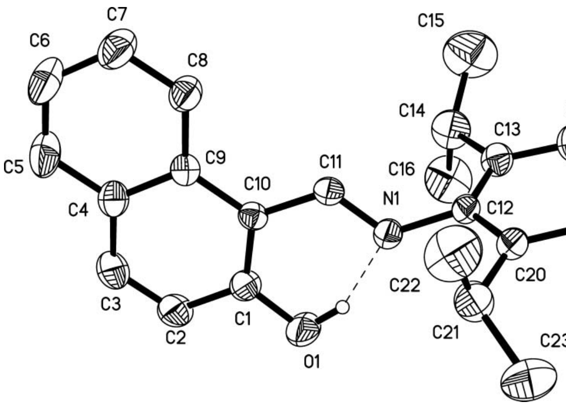

Figure 1
View of (I) with the atom-numbering scheme and 30% probability displacement ellipsoids. Only one H atom participating in the intramolecular O—H···N hydrogen bond (dashed line) is shown; the rest have been omitted for clarity. For the disordered atoms, only the major components are shown.

The two methyl atoms, C15 and C16, in one of the isopropyl groups show positional disorder. They were refined as two groups sharing the same C14 atom. The C14—C15, C14—C15′, C14—C16 and C14—C16′ distances were restrained to a value of 1.53 (1) Å. The displacement parameters of the disordered C atoms were also restrained weakly to be approximately isotropic. Accordingly, the H atom of C14 was added in two positions. The resulting occupancy factors for the two disordered groups of atoms were 0.66 (3) and 0.34 (3), respectively. The aromatic [C—H = 0.93 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C)] and alkyl [C—H = 0.96 Å and $U_{\rm iso}$(H) = $1.5U_{\rm eq}$(C)] H atoms and atom H21 [C21—H21 = 0.98 Å and $U_{\rm iso}$(H21) = $1.2U_{\rm eq}$(C21)] were positioned geometrically and included in the refinement in the riding-model approximation. Hydroxy atom H1 was located in a Fourier difference map and refined isotropically with an O—H distance restraint of 0.82 (2) Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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