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N,*N*-Diethyl-2-(2′-hydroxy-1,1′-binaphthalen-2-yloxy)acetamide

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.055
wR factor = 0.164
Data-to-parameter ratio = 13.6

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

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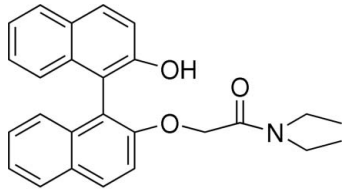
The title compound, $C_{26}H_{25}NO_3$, is a BINOL (1,1′-2,2′-binaphthol) derivative. In the structure, there is one intramolecular O—H···O hydrogen bond.

Comment

The title compound, (I), is a new derivative of 1,1′-2,2′-binaphthol. It is of interest to us since binaphthyl molecules are considered to be promising ligands for chiral recognition and catalysis (Knof & Zelewsky, 1999; Kagan & Riant, 1992).



(I)

In the crystal structure of (I), the two naphthalene ring systems are almost perpendicular to each other, with an average dihedral angle of 108.7° (Fig. 1). There is also an intramolecular O—H···O hydrogen bond (Table 1).

Experimental

Compound (I) was prepared according to a literature method (Fan *et al.*, 2000; Zhang *et al.*, 2003), which gave a yield of 54%. Single crystals were obtained by slow evaporation of a $CHCl_3$ solution over a period of several days.

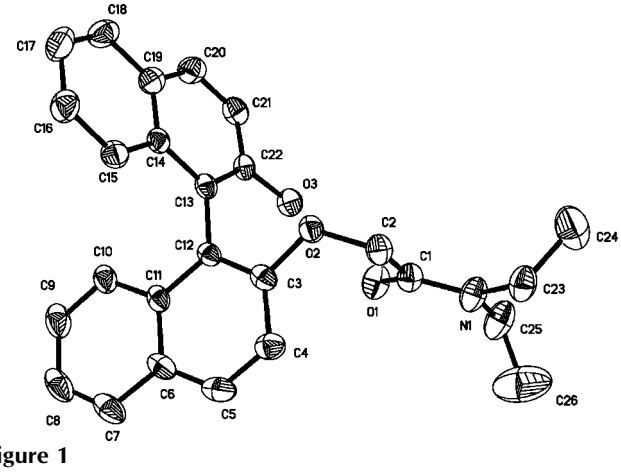


Figure 1
The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted.

Crystal data

$C_{26}H_{25}NO_3$
M_r = 399.47
Monoclinic, $P2_1/c$
a = 11.361 (2) Å
b = 10.304 (3) Å
c = 18.355 (4) Å
β = 103.242 (3)°
V = 2091.5 (9) Å^3
Z = 4
D_x = 1.269 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
Block, colorless
0.42 × 0.38 × 0.21 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*DENZO-SMN*; Otwinowski & Minor, 1997)
T_{min} = 0.966, T_{max} = 0.983
10716 measured reflections
3688 independent reflections
1767 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.164
S = 1.01
3688 reflections
271 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.9737P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O1	0.82	2.17	2.749 (3)	128

H atoms were positioned geometrically (O—H = 0.82, C—H = 0.93–0.97 Å) and refined as riding, with U_{iso}(H) = 1.5U_{eq}(O) and 1.2 or 1.5 times U_{eq}(C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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