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(*S*)-2,2′-Diethoxy-1,1′-binaphthyl

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.097
Data-to-parameter ratio = 9.3

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

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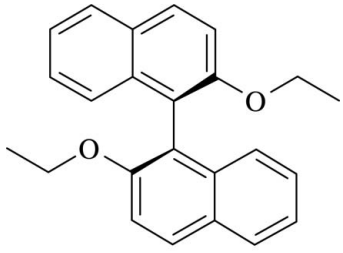
The title molecule, $C_{24}H_{22}O_2$, contains two planar naphthyl ring systems. The torsion angle around the the central C—C bond is 111.3 (2)° implying a *transoid* conformation with respect to the two ethoxy substituents. Only weak intermolecular interactions are present in the crystal structure.

Comment

The structure of (*S*)-2,2′-diethoxy-1,1′-binaphthyl, (I), was determined as part of a study of several binaphthalene derivatives as possible candidates for second-order non-linear optics (Deussen, Hendricks *et al.*, 1996; Deussen *et al.*, 1998), as well as chiral dopants for nematic liquid crystals (Deussen, Shibaev *et al.*, 1996; Shibaev *et al.* 1997). The molecules studied for second-order non-linear optics had electron-acceptor groups at their 6,6′-positions to increase polarizability. The title compound is thus not expected to exhibit second-order optical properties although the crystal structure requirement of non-centrosymmetry is fulfilled.



(I)

The molecular structure is depicted in Fig. 1. The absolute configuration is known to be *S*, but the chirality could not be determined based on the diffraction data (Friedel pairs were merged). As expected, each of the two naphthyl ring systems is planar. The molecule is twisted around the central C1—C13 bond with a torsion angle C2—C1—C13—C14 of 111.3 (2)°. This conformation prevents close interactions between ring systems in neighboring molecules. There are no remarkable short intermolecular distances in the structure. Thus, the intermolecular attractions appear to be rather weak, which is in accordance with the observed low melting point (*ca* 412 K).

Experimental

(*S*)-2,2′-Diethoxy-1,1′-binaphthyl was prepared as previously reported (Deussen, Hendricks *et al.*, 1996). Crystals for X-ray analysis were obtained by crystallization from a solution in ligroin.

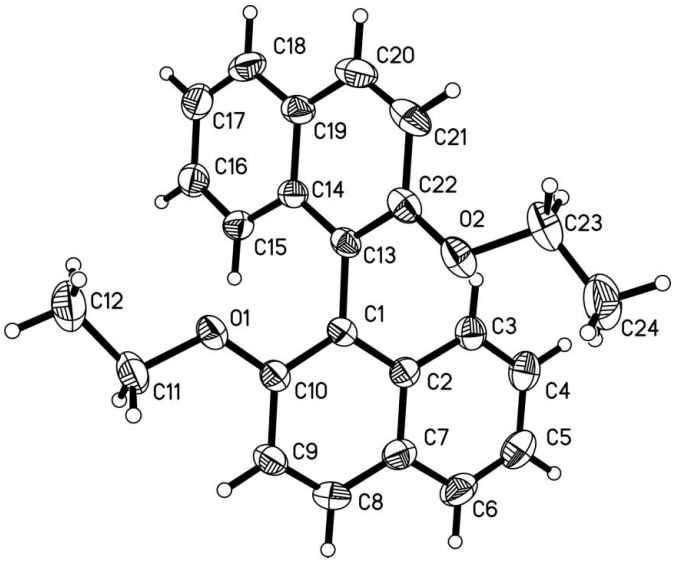


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radii.

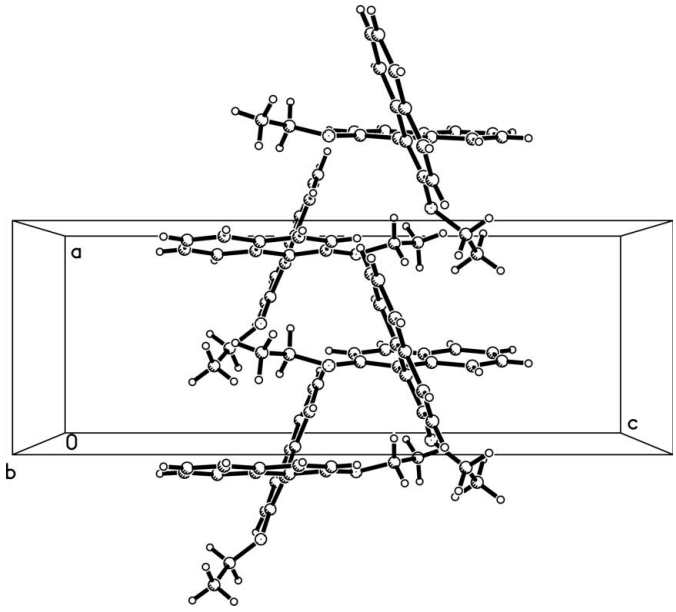


Figure 2
Packing, viewed along the *b*-axis direction.

Crystal data

$C_{24}H_{22}O_2$
M_r = 342.42
Orthorhombic, $P2_12_12_1$
a = 7.5637 (5) Å
b = 11.5604 (7) Å
c = 21.3353 (13) Å
V = 1865.5 (2) Å^3
Z = 4
D_x = 1.219 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4698 reflections
θ = 1.9–26.4°
μ = 0.08 mm^{-1}
T = 295 (2) K
Prism, colorless
0.38 × 0.20 × 0.14 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.878, T_{max} = 0.989
10849 measured reflections
2214 independent reflections
1719 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 26.4°
$h = -9 \rightarrow 9$
$k = -14 \rightarrow 13$
$l = -26 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.097
S = 1.04
2214 reflections
238 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 0.1176P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.018 (2)

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

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* and *PLATON*.

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