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# (±)-1-{[(4-Methoxybenzylidene)-amino](4-methoxyphenyl)methyl}-2-naphthol

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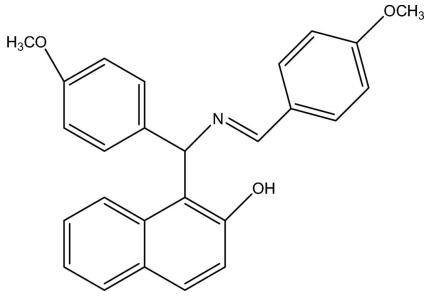
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.071; $wR$ factor = 0.156; data-to-parameter ratio = 13.1.

The title compound, $C_{26}H_{23}NO_3$, is a key intermediate used in the synthesis of 1-[amino(4-methoxyphenyl)methyl]-2-naphthol, which has been found to be a potent chiral catalyst in the addition reactions of dialkylzinc compounds with aldehydes. The $\pi$-conjugated system formed by the methoxybenzylidene–imine tautomer is essentially planar. An intramolecular O—H···N hydrogen bond is formed between the hydroxyl OH group attached to the naphthalene group and the Schiff base N atom. The crystal packing is stabilized by van der Waals forces.

## Related literature

For related literature, see: Szatmari *et al.* (2003).




## Experimental

### Crystal data

$C_{26}H_{23}NO_3$
$M_r$ = 397.45
Monoclinic, $P2_1/c$
$a$ = 20.790 (5) Å
$b$ = 10.717 (3) Å
$c$ = 9.470 (2) Å
$\beta$ = 102.952 (4)°
$V$ = 2056.4 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 298 (2) K
0.46 × 0.45 × 0.16 mm

### Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.963, $T_{max}$ = 0.987
10108 measured reflections
3595 independent reflections
3150 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.156
$S$ = 1.22
3594 reflections
274 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3···N1 | 0.82 | 1.82 | 2.544 (3) | 146 |

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2180).

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