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(*E*)-4-{[(4-Methoxynaphthalen-1-yl)methylidene]amino}phenol

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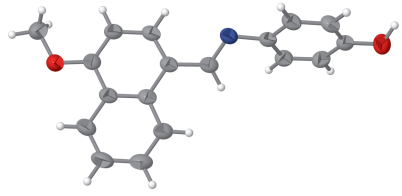
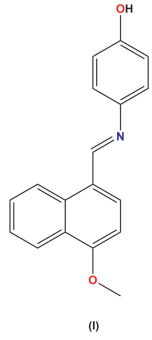
The title Schiff base compound, $C_{18}H_{15}NO_2$, was synthesized *via* the condensation reaction of 4-hydroxy aniline and 4-methoxy-1-naphthaldehyde in ethanol. The dihedral angle between the phenol ring and the mean plane of the naphthalene ring system is 75.81 (6)°. In the crystal, the molecules are linked by O—H···N and C—H···O hydrogen bonds, enclosing $R_3^3(18)$ ring motifs and forming zigzag chains propagating along the *c*-axis direction. The chains are linked *via* C—H···π interactions forming slabs lying parallel to the *ac* plane.

3D view



Chemical scheme



(I)

Structure description

Schiff bases exhibit a wide range of biological activities (Djabbour *et al.*, 2025; Villar *et al.*, 2004). They have applications in the field of water treatment as they have a great capacity for complexation of transition metals (Boudraa *et al.*, 2023; Kalcher *et al.*, 1995). Their use as corrosion inhibitors (*e.g.*, Boudraa *et al.*, 2023) reveal their importance in this field too. Herein, we report on the synthesis and crystal structure of the title compound, $C_{18}H_{15}NO_2$ (**I**).

The molecular structure of compound (**I**) is illustrated in Fig. 1. The configuration about the N1═C12 azomethine bond is *E*. The –C═N– bond length [1.282 (2) Å] is a little longer than the bond lengths observed in related compounds, such as (*E*)-1-(4-methoxynaphthalen-1-yl)-*N*-phenylmethanimine (**II**) [1.264 (4) Å; Linden *et al.*, 1989] and (*E*)-2-{[(4-methoxynaphthalen-1-yl)methylene]amino}-4-methylphenol (**III**)

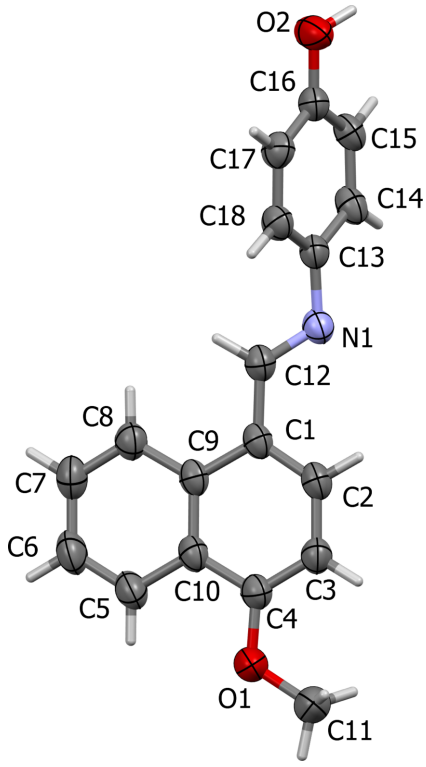


Figure 1
A view of the molecular structure of compound (**I**). The displacement ellipsoids are drawn at the 50% probability level.

[1.274 (2) Å; Yahiaoui *et al.*, 2023]. A search of the Cambridge Structural Database (CSD, Version 6.01; last update May 2026; Groom *et al.*, 2016) for the length of the azomethine bond of structures with the benzylideneaniline substructure gave 1601 hits (Filters: $R \leq 0.05$, no disorder, no ions, no polymers, single crystals and organics only). An analysis using *Mercury* (Macrae *et al.*, 2020) gave an average value for the –C═N– bond length of 1.277 (15) Å, with a median value of 1.278 Å. Hence, the N1═C12 bond length in (**I**) is normal.

The dihedral angle between the phenol ring (C13–C18) and the mean plane of the naphthalene ring system (C1–C10; r.m.s. deviation 0.013 Å) in (**I**) is 75.81 (6)°. In compound (**II**) the corresponding dihedral angle is 64.33 (12)°, while in compound (**III**) the same dihedral angle is smaller, at 33.41 (4)° probably due to the presence of an intramolecular O—H···N hydrogen bond.

In the crystal of (**I**), the molecules are linked by O—H···N hydrogen bonds to form zigzag chains propagating along the *c*-axis direction (Fig. 2). The chains are consolidated by C—H···O hydrogen bonds, so enclosing $R_3^3(18)$ ring motifs (Fig. 2, Table 1). The chains are linked by C—H···π interactions forming slabs lying parallel to the *ac* plane (Fig. 3, Table 1). The slabs stack along the *b*-axis direction and there are no significant inter-planar interactions present.

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

*Cg*1 and *Cg*2 are the centroids of the naphthalene ring system (C1–C10) and the phenol ring (C13–C18), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1···N1^{i}	0.91 (3)	1.97 (3)	2.849 (2)	160 (3)
C11—H11*A*···O2^{ii}	0.97	2.53	3.409 (2)	150
C14—H14···*Cg*2^{iii}	0.94	2.90	3.627 (2)	135
C18—H18···*Cg*1^{iv}	0.94	2.82	3.745 (2)	170

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

Synthesis and crystallization

Equimolar amounts of 4-hydroxy aniline (0.109 g, 0.01 mmol) and 4-methoxy naphthaldehyde (0.186 g, 0.01 mmol) were mixed in absolute ethanol (30 ml) and refluxed under stirring for 4 h. After cooling to room temperature, the solvent was allowed to evaporate slowly, yielding yellow needle-like crystals of (**I**).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

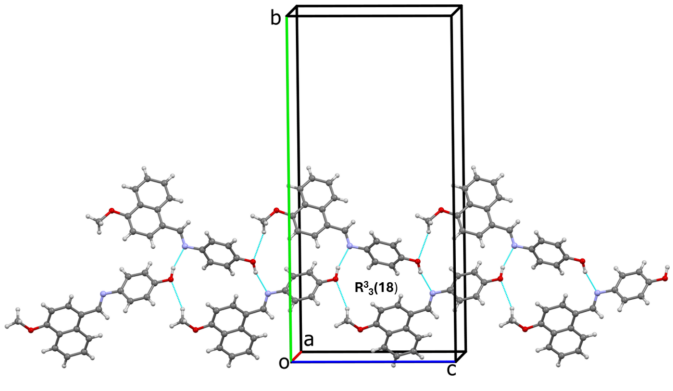


Figure 2
A partial view along the *a*-axis of the crystal structure of compound **I**, illustrating the formation of the zigzag chain *via* O—H···N and C—H···O hydrogen bonds and the formation of the $R_3^3(18)$ ring motifs (Table 1). The various hydrogen bonds are shown as cyan dashed lines.

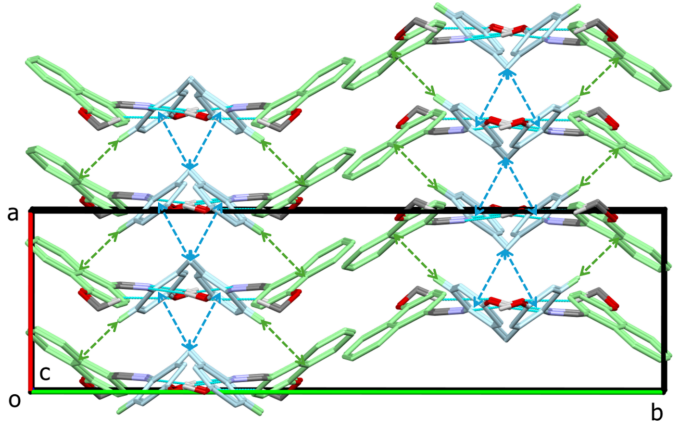


Figure 3
A view along the *c*-axis of the crystal packing of compound **I**. The C—H···π interactions are shown as dashed double arrows (see Table 1; naphthalene ring system is pale green and the phenol ring is pale blue).

Acknowledgements

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{15}NO_2$
M_r	277.31
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	250
a, b, c (Å)	7.8365 (3), 27.460 (1), 13.0741 (5)
V (Å^3)	2813.43 (18)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.69
Crystal size (mm)	0.54 × 0.24 × 0.09
Data collection	
Diffractometer	Stoe Stadivari
Absorption correction	Analytical (*X-RED32* and *LANA*; Stoe, 2025)
T_{min}, T_{max}	0.682, 0.938
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17634, 2477, 2243
R_{int}	0.057
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.131, 1.01
No. of reflections	2477
No. of parameters	195
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.25

Computer programs: *X-AREA Pilatus3_SV*, *X-AREA* and *LANA* (Stoe, 2025), *SHELXT2019/3* (Sheldrick, 2015*a*), *Mercury* (Macrae *et al.*, 2020), *SHELXL2019/3* (Sheldrick, 2015*b*), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

full crystallographic data

IUCrData (2026). **11**, x260855 [https://doi.org/10.1107/S2414314626008552]

(*E*)-4-{[(4-Methoxynaphthalen-1-yl)methylidene]amino}phenol

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(*E*)-4-{[(4-Methoxynaphthalen-1-yl)methylidene]amino}phenol

Crystal data

$C_{18}H_{15}NO_2$
M_r = 277.31
Orthorhombic, *Pbca*
a = 7.8365 (3) Å
b = 27.460 (1) Å
c = 13.0741 (5) Å
V = 2813.43 (18) Å^3
Z = 8
F(000) = 1168
D_x = 1.309 Mg m^{-3}
Cu *Kα* radiation, λ = 1.54186 Å
Cell parameters from 30029 reflections
θ = 4.7–67.1°
μ = 0.69 mm^{-1}
T = 250 K
Needle, yellow
0.54 × 0.24 × 0.09 mm

Data collection

Stoe Stadivari diffractometer
Radiation source: Primux 100 micro
Graded multilayer mirror monochromator
Detector resolution: 5.81 pixels mm^{-1}
rotation method, ω scans
Absorption correction: analytical (X-Red32 and *LANA*; Stoe, 2025)
T_{min} = 0.682, T_{max} = 0.938
17634 measured reflections
2477 independent reflections
2243 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 66.9°, θ_{min} = 4.7°
h = −3→9
k = −32→27
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.131
S = 1.01
2477 reflections
195 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0836P)^2 + 0.6531P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The hydroxyl H atom (H1) was located in a difference Fourier map and freely refined. The C-bound hydrogen atoms were placed geometrically (C—H = 0.94–0.97 Å) and allowed to ride on their parent atoms with U_{iso}(H) = 1.5U_{eq}(*C*-methyl) and 1.2U_{eq}(C) for other H atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.54483 (17)	0.42260 (4)	−0.11052 (8)	0.0607 (3)
O2	0.50176 (18)	0.27526 (4)	0.74559 (9)	0.0631 (4)
H1	0.535 (4)	0.2440 (11)	0.759 (2)	0.112 (9)*
N1	0.56304 (15)	0.31870 (4)	0.33044 (9)	0.0431 (3)
C1	0.57080 (17)	0.37828 (5)	0.19453 (11)	0.0408 (3)
C2	0.48289 (18)	0.35110 (5)	0.12373 (11)	0.0438 (3)
H2	0.429306	0.322240	0.145278	0.053*
C3	0.46995 (19)	0.36462 (5)	0.02107 (11)	0.0456 (3)
H3	0.408485	0.345058	−0.025015	0.055*
C4	0.54710 (19)	0.40648 (5)	−0.01231 (11)	0.0448 (4)
C5	0.7243 (2)	0.47925 (5)	0.02372 (13)	0.0544 (4)
H5	0.717067	0.488614	−0.045305	0.065*
C6	0.8157 (2)	0.50699 (6)	0.09119 (14)	0.0611 (5)
H6	0.871221	0.535300	0.068213	0.073*
C7	0.8272 (2)	0.49353 (5)	0.19402 (14)	0.0566 (4)
H7	0.890171	0.512896	0.239741	0.068*
C8	0.74786 (19)	0.45251 (5)	0.22859 (12)	0.0477 (4)
H8	0.756775	0.444017	0.298037	0.057*
C9	0.65200 (17)	0.42243 (4)	0.16155 (11)	0.0404 (3)
C10	0.64038 (18)	0.43649 (4)	0.05746 (11)	0.0423 (3)
C11	0.4544 (3)	0.39390 (7)	−0.18289 (14)	0.0765 (6)
H11C	0.462324	0.408915	−0.249878	0.115*
H11B	0.335501	0.391672	−0.162765	0.115*
H11A	0.503581	0.361505	−0.185446	0.115*
C12	0.57358 (18)	0.36320 (5)	0.30148 (11)	0.0433 (3)
H12	0.583650	0.387430	0.351919	0.052*
C13	0.55024 (17)	0.30924 (5)	0.43688 (10)	0.0404 (3)
C14	0.64259 (18)	0.27075 (5)	0.47837 (11)	0.0457 (4)
H14	0.712289	0.251745	0.435586	0.055*
C15	0.63350 (19)	0.26002 (5)	0.58132 (12)	0.0461 (4)
H15	0.701496	0.234978	0.608536	0.055*
C16	0.52446 (19)	0.28599 (5)	0.64513 (11)	0.0453 (4)
C17	0.4292 (2)	0.32384 (5)	0.60349 (11)	0.0486 (4)
H17	0.353863	0.341496	0.645387	0.058*
C18	0.44399 (19)	0.33576 (5)	0.50134 (11)	0.0448 (3)
H18	0.381461	0.362145	0.474999	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0941 (9)	0.0422 (6)	0.0456 (6)	−0.0098 (5)	−0.0054 (5)	0.0026 (4)

O2	0.0974 (9)	0.0459 (6)	0.0459 (6)	0.0143 (6)	0.0037 (5)	0.0037 (5)
N1	0.0487 (7)	0.0341 (6)	0.0465 (7)	−0.0005 (5)	0.0025 (5)	0.0007 (5)
C1	0.0435 (7)	0.0305 (6)	0.0484 (8)	0.0030 (5)	0.0021 (5)	0.0000 (5)
C2	0.0469 (7)	0.0312 (6)	0.0534 (8)	−0.0015 (6)	0.0022 (6)	0.0008 (6)
C3	0.0521 (8)	0.0352 (7)	0.0496 (8)	−0.0023 (6)	−0.0043 (6)	−0.0032 (6)
C4	0.0550 (8)	0.0337 (7)	0.0459 (8)	0.0037 (6)	0.0005 (6)	−0.0003 (6)
C5	0.0684 (10)	0.0363 (7)	0.0585 (9)	−0.0048 (7)	0.0056 (7)	0.0038 (6)
C6	0.0711 (11)	0.0369 (8)	0.0752 (11)	−0.0145 (7)	0.0048 (8)	0.0013 (7)
C7	0.0594 (10)	0.0381 (7)	0.0723 (11)	−0.0078 (7)	−0.0045 (7)	−0.0074 (7)
C8	0.0522 (8)	0.0368 (7)	0.0541 (8)	0.0003 (6)	−0.0037 (6)	−0.0028 (6)
C9	0.0418 (7)	0.0293 (6)	0.0501 (8)	0.0045 (5)	0.0020 (6)	−0.0018 (5)
C10	0.0470 (8)	0.0300 (6)	0.0500 (8)	0.0026 (5)	0.0034 (6)	−0.0014 (5)
C11	0.1276 (18)	0.0512 (10)	0.0508 (10)	−0.0136 (10)	−0.0176 (10)	0.0001 (7)
C12	0.0464 (8)	0.0342 (7)	0.0493 (8)	−0.0001 (6)	−0.0001 (6)	−0.0012 (6)
C13	0.0452 (7)	0.0315 (6)	0.0446 (7)	−0.0036 (5)	−0.0014 (5)	−0.0010 (5)
C14	0.0477 (8)	0.0330 (7)	0.0563 (9)	0.0034 (5)	0.0086 (6)	0.0022 (6)
C15	0.0499 (8)	0.0330 (7)	0.0553 (8)	0.0031 (6)	0.0001 (6)	0.0070 (6)
C16	0.0583 (8)	0.0339 (7)	0.0437 (8)	−0.0025 (6)	−0.0039 (6)	−0.0011 (5)
C17	0.0601 (9)	0.0389 (7)	0.0467 (8)	0.0083 (6)	−0.0005 (7)	−0.0064 (6)
C18	0.0519 (8)	0.0346 (7)	0.0480 (8)	0.0077 (6)	−0.0045 (6)	−0.0010 (6)

Geometric parameters (Å, º)

O1—C4	1.3583 (18)	C7—C8	1.364 (2)
O1—C11	1.421 (2)	C7—H7	0.9400
O2—C16	1.3578 (18)	C8—C9	1.420 (2)
O2—H1	0.91 (3)	C8—H8	0.9400
N1—C12	1.2820 (18)	C9—C10	1.417 (2)
N1—C13	1.4192 (18)	C11—H11C	0.9700
C1—C2	1.374 (2)	C11—H11B	0.9700
C1—C9	1.4354 (18)	C11—H11A	0.9700
C1—C12	1.4585 (19)	C12—H12	0.9400
C2—C3	1.396 (2)	C13—C18	1.391 (2)
C2—H2	0.9400	C13—C14	1.3911 (19)
C3—C4	1.370 (2)	C14—C15	1.380 (2)
C3—H3	0.9400	C14—H14	0.9400
C4—C10	1.430 (2)	C15—C16	1.391 (2)
C5—C6	1.368 (2)	C15—H15	0.9400
C5—C10	1.416 (2)	C16—C17	1.391 (2)
C5—H5	0.9400	C17—C18	1.380 (2)
C6—C7	1.397 (2)	C17—H17	0.9400
C6—H6	0.9400	C18—H18	0.9400
C4—O1—C11	117.08 (12)	C9—C10—C5	119.68 (13)
C16—O2—H1	110.3 (19)	C9—C10—C4	119.23 (12)
C12—N1—C13	117.95 (12)	C5—C10—C4	121.08 (14)
C2—C1—C9	118.59 (13)	O1—C11—H11C	109.5
C2—C1—C12	119.94 (12)	O1—C11—H11B	109.5

C9—C1—C12	121.41 (12)	H11C—C11—H11B	109.5
C1—C2—C3	122.64 (13)	O1—C11—H11A	109.5
C1—C2—H2	118.7	H11C—C11—H11A	109.5
C3—C2—H2	118.7	H11B—C11—H11A	109.5
C4—C3—C2	119.82 (13)	N1—C12—C1	123.56 (13)
C4—C3—H3	120.1	N1—C12—H12	118.2
C2—C3—H3	120.1	C1—C12—H12	118.2
O1—C4—C3	124.66 (13)	C18—C13—C14	118.23 (13)
O1—C4—C10	114.96 (12)	C18—C13—N1	122.73 (12)
C3—C4—C10	120.38 (13)	C14—C13—N1	118.99 (12)
C6—C5—C10	120.26 (15)	C15—C14—C13	121.05 (13)
C6—C5—H5	119.9	C15—C14—H14	119.5
C10—C5—H5	119.9	C13—C14—H14	119.5
C5—C6—C7	120.45 (14)	C14—C15—C16	120.49 (13)
C5—C6—H6	119.8	C14—C15—H15	119.8
C7—C6—H6	119.8	C16—C15—H15	119.8
C8—C7—C6	120.54 (15)	O2—C16—C17	118.07 (13)
C8—C7—H7	119.7	O2—C16—C15	123.33 (13)
C6—C7—H7	119.7	C17—C16—C15	118.56 (13)
C7—C8—C9	121.15 (15)	C18—C17—C16	120.74 (13)
C7—C8—H8	119.4	C18—C17—H17	119.6
C9—C8—H8	119.4	C16—C17—H17	119.6
C10—C9—C8	117.92 (12)	C17—C18—C13	120.84 (13)
C10—C9—C1	119.34 (12)	C17—C18—H18	119.6
C8—C9—C1	122.72 (13)	C13—C18—H18	119.6

C9—C1—C2—C3	0.2 (2)	C6—C5—C10—C4	−178.70 (15)
C12—C1—C2—C3	177.47 (13)	O1—C4—C10—C9	−179.24 (12)
C1—C2—C3—C4	0.1 (2)	C3—C4—C10—C9	0.0 (2)
C11—O1—C4—C3	0.6 (2)	O1—C4—C10—C5	−0.7 (2)
C11—O1—C4—C10	179.71 (16)	C3—C4—C10—C5	178.48 (14)
C2—C3—C4—O1	178.93 (13)	C13—N1—C12—C1	−173.88 (12)
C2—C3—C4—C10	−0.2 (2)	C2—C1—C12—N1	29.7 (2)
C10—C5—C6—C7	−0.1 (3)	C9—C1—C12—N1	−153.10 (13)
C5—C6—C7—C8	0.2 (3)	C12—N1—C13—C18	43.94 (19)
C6—C7—C8—C9	0.1 (2)	C12—N1—C13—C14	−138.50 (14)
C7—C8—C9—C10	−0.4 (2)	C18—C13—C14—C15	−2.0 (2)
C7—C8—C9—C1	178.18 (14)	N1—C13—C14—C15	−179.68 (12)
C2—C1—C9—C10	−0.44 (19)	C13—C14—C15—C16	3.4 (2)
C12—C1—C9—C10	−177.64 (12)	C14—C15—C16—O2	175.76 (14)
C2—C1—C9—C8	−178.98 (13)	C14—C15—C16—C17	−1.9 (2)
C12—C1—C9—C8	3.8 (2)	O2—C16—C17—C18	−178.60 (13)
C8—C9—C10—C5	0.42 (19)	C15—C16—C17—C18	−0.8 (2)
C1—C9—C10—C5	−178.19 (13)	C16—C17—C18—C13	2.1 (2)
C8—C9—C10—C4	178.96 (12)	C14—C13—C18—C17	−0.7 (2)
C1—C9—C10—C4	0.35 (19)	N1—C13—C18—C17	176.85 (13)
C6—C5—C10—C9	−0.2 (2)		

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the naphthalene ring system (C1–C10) and the phenol ring (C13–C18), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1···N1^{i}	0.91 (3)	1.97 (3)	2.849 (2)	160 (3)
C11—H11*A*···O2^{ii}	0.97	2.53	3.409 (2)	150
C14—H14···*Cg*2^{iii}	0.94	2.90	3.627 (2)	135
C18—H18···*Cg*1^{iv}	0.94	2.82	3.745 (2)	170

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