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# 4-*tert*-Butyl-2-{[(*E*)-2,6-diisopropylphenylimino]methyl}-6-(1-phenylethyl)phenol

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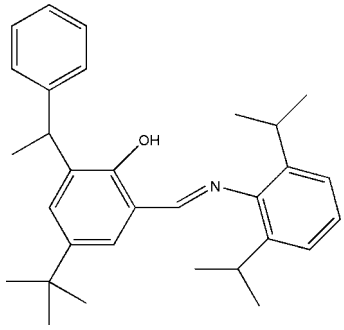
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.005 Å; disorder in main residue; $R$ factor = 0.038; $wR$ factor = 0.105; data-to-parameter ratio = 7.9.

The title compound, $C_{31}H_{39}NO$, was prepared by the condensation of 5-*tert*-butyl-2-hydroxy-3-(1-phenylethyl)-benzaldehyde with 2,6-diisopropylphenylamine in refluxing ethanol. The phenol ring and the phenylimino ring are approximately perpendicular, forming a dihedral angle of 81.5 (3)°. The phenyl ring makes a dihedral angle of 75.2 (2)° with the phenol ring and also makes a dihedral angle of 62.9 (3)° with the phenylimino ring. The molecular structure is stabilized by an intramolecular O—H···N hydrogen bond linking the phenol OH group and the phenylimino N atom. One of the isopropyl groups is disordered over two positions; the site occupancies are 0.55 and 0.45.

## Related literature

For related literature, see: Gibson & Spitzmesser (2003); Ittel & Johnson (2000); Shriner *et al.* (1946).




## Experimental

### Crystal data

$C_{31}H_{39}NO$
$M_r$ = 441.63
Orthorhombic, $Pca2_1$
$a$ = 25.273 (4) Å
$b$ = 9.5496 (18) Å
$c$ = 11.115 (2) Å
$V$ = 2682.6 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 294 (2) K
0.24 × 0.20 × 0.16 mm

### Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.974, $T_{max}$ = 0.990
13332 measured reflections
2505 independent reflections
1964 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.105
$S$ = 1.06
2505 reflections
319 parameters
41 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.13 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.12 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N1 | 0.93 (4) | 1.79 (4) | 2.620 (3) | 147 (3) |

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2047).

## References

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o4400 [ **doi:10.1107/S1600536807051306** ]

# 4-*tert*-Butyl-2-{[(*E*)-2,6-diisopropylphenylimino]methyl}-6-(1-phenylethyl)phenol

**J. Cui, M. Zhang, J. Zhu, N. Cui and B. Liu**

## Comment

Late-metal catalysts bearing salicylaldiminato-type ligands play an important role in the catalytic oligomerization and polymerization of olefins (Ittel *et al.*, 2000). Increasing the size of the imino substituent and the *o*-phenoxy substituent has a pronounced effect on the activity of the catalyst and the molecular weight of the polymer (Gibson *et al.*, 2003). We have recently prepared a novel ligand, (I), and report its crystal structure here.

The molecular structure of (I) is shown in Fig. 1. In (I) the phenyl ring and the phenoxy ring form a dihedral angle of 75.18 (1)°, the phenylimino ring is nearly perpendicular to the phenoxy ring, with a dihedral angle of 81.51 (2)°. The dihedral angle between the phenyl and the phenylimino ring is 62.88 (1)°. Three C atoms of isopropyl attaching to the phenylimino ring are disordered in two locations with 55% and 45% probabilities. An intramolecular hydrogen bond is formed between the hydroxyl group and the N atom stabilizing the crystal structure.

## Experimental

2,6-Diisopropylaniline (3.94 g, 22.2 mmol) was added *via* syringe to a solution of 5-*tert*-Butyl-2-hydroxy-3-(1-phenylethyl)-benzaldehyde (6.26 g, 22.2 mmol) in EtOH (100 ml). Formic acid (0.01 g, 0.22 mmol) was added and the solution refluxed for 20 h. The solution was dried over magnesium sulfate, filtered and the volatiles removed under reduced pressure. Extraction into pentane (5 ml) followed by cooling to 243 K afforded yellow crystals of (I) (yield 76%). Spectroscopic analysis: IR (KBr, ν, $cm^{-1}$): 3055.8, 3027.2, 2965.6, 2871.9, 1621.5, 1591.1, 1460.4, 1361.9, 1269.7, 1176.9, 855.7; $^1$H NMR ($CDCl_3$, δ, p.p.m.): 1.188 (s, 12H), 1.305 (s, 9H), 1.692 (s, 3H), 3.021 (s, 2H), 4.756 (s, 1H), 7.182–7.369 (m, 10H), 8.287 (s, 1H), 13.146 (s, 1H)

## Refinement

Except the hydroxyl H atom, all H atoms were positioned geometrically (C—H=0.93–0.97 Å) and refined as riding. $U_{iso}$(H) values are equal to 1.2$U_{eq}$(carrier atom). In absence of significant anomalous dispersion effects, Friedel-pair reflections were merged prior to refinement.

## Figures

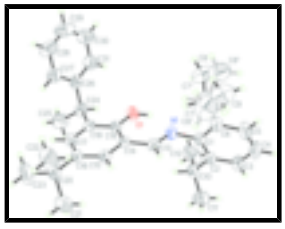


Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

## 4-*tert*-Butyl-2-{[(*E*)-2,6-diisopropylphenylimino]methyl}-6-(1-phenylethyl)phenol

### *Crystal data*

| | |
|---|---|
| $C_{31}H_{39}NO$ | $D_x = 1.093$ Mg m$^{-3}$ |
| $M_r = 441.63$ | Melting point: 400 K |
| Orthorhombic, $Pca2_1$ | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 25.273$ (4) Å | Cell parameters from 3934 reflections |
| $b = 9.5496$ (18) Å | $\theta = 2.3$–$24.1$º |
| $c = 11.115$ (2) Å | $\mu = 0.07$ mm$^{-1}$ |
| $V = 2682.6$ (8) Å$^3$ | $T = 294$ (2) K |
| $Z = 4$ | Block, yellow |
| $F_{000} = 960$ | 0.24 × 0.20 × 0.16 mm |

### *Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD diffractometer | 2505 independent reflections |
| Radiation source: fine-focus sealed tube | 1964 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.039$ |
| $T = 294$(2) K | $\theta_{max} = 25.0$º |
| φ and ω scans | $\theta_{min} = 2.1$º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h = -19 \rightarrow 30$ |
| $T_{min} = 0.974$, $T_{max} = 0.990$ | $k = -11 \rightarrow 9$ |
| 13332 measured reflections | $l = -11 \rightarrow 13$ |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.105$ | $w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.4436P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.06$ | $(\Delta/\sigma)_{max} = 0.003$ |
| 2505 reflections | $\Delta\rho_{max} = 0.13$ e Å$^{-3}$ |
| 319 parameters | $\Delta\rho_{min} = -0.12$ e Å$^{-3}$ |
| 41 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| O1 | 0.44217 (8) | 0.0843 (2) | 0.9096 (2) | 0.0504 (5) | |
| H1 | 0.4093 (15) | 0.115 (4) | 0.937 (4) | 0.076* | |
| N1 | 0.34993 (8) | 0.2094 (3) | 0.9030 (2) | 0.0441 (6) | |
| C1 | 0.29497 (10) | 0.2202 (3) | 0.9371 (3) | 0.0420 (7) | |
| C2 | 0.26067 (11) | 0.1171 (3) | 0.8930 (3) | 0.0456 (7) | |
| C3 | 0.20812 (12) | 0.1214 (4) | 0.9313 (3) | 0.0571 (9) | |
| H3A | 0.1845 | 0.0538 | 0.9039 | 0.069* | |
| C4 | 0.19064 (13) | 0.2234 (4) | 1.0087 (4) | 0.0647 (10) | |
| H4A | 0.1555 | 0.2246 | 1.0331 | 0.078* | |
| C5 | 0.22512 (13) | 0.3240 (4) | 1.0501 (3) | 0.0597 (9) | |
| H5A | 0.2126 | 0.3936 | 1.1012 | 0.072* | |
| C6 | 0.27828 (12) | 0.3240 (3) | 1.0173 (3) | 0.0489 (8) | |
| C7 | 0.31638 (13) | 0.4301 (4) | 1.0708 (3) | 0.0585 (9) | 0.55 |
| H7A | 0.3432 | 0.4506 | 1.0096 | 0.070* | 0.55 |
| C8 | 0.3442 (4) | 0.3728 (10) | 1.1771 (9) | 0.093 (3) | 0.55 |
| H8A | 0.3612 | 0.2864 | 1.1558 | 0.140* | 0.55 |
| H8B | 0.3192 | 0.3560 | 1.2404 | 0.140* | 0.55 |
| H8C | 0.3703 | 0.4387 | 1.2042 | 0.140* | 0.55 |
| C9 | 0.2903 (4) | 0.5695 (8) | 1.1056 (11) | 0.094 (3) | 0.55 |
| H9A | 0.2724 | 0.6078 | 1.0370 | 0.141* | 0.55 |
| H9B | 0.3169 | 0.6340 | 1.1324 | 0.141* | 0.55 |
| H9C | 0.2653 | 0.5539 | 1.1692 | 0.141* | 0.55 |
| C7' | 0.31638 (13) | 0.4301 (4) | 1.0708 (3) | 0.0585 (9) | 0.45 |
| H7'A | 0.3517 | 0.4052 | 1.0413 | 0.070* | 0.45 |
| C8' | 0.3184 (5) | 0.4162 (15) | 1.2099 (8) | 0.101 (4) | 0.45 |
| H8'A | 0.3426 | 0.4838 | 1.2420 | 0.152* | 0.45 |
| H8'B | 0.3299 | 0.3237 | 1.2311 | 0.152* | 0.45 |
| H8'C | 0.2837 | 0.4325 | 1.2426 | 0.152* | 0.45 |
| C9' | 0.3053 (5) | 0.5723 (10) | 1.0256 (14) | 0.101 (4) | 0.45 |
| H9'A | 0.3053 | 0.5715 | 0.9392 | 0.152* | 0.45 |
| H9'B | 0.3320 | 0.6356 | 1.0540 | 0.152* | 0.45 |
| H9'C | 0.2712 | 0.6023 | 1.0540 | 0.152* | 0.45 |
| C10 | 0.27988 (12) | 0.0008 (3) | 0.8111 (3) | 0.0538 (8) | |
| H10A | 0.3106 | 0.0365 | 0.7670 | 0.065* | |
| C11 | 0.23939 (16) | −0.0449 (5) | 0.7194 (4) | 0.0823 (13) | |
| H11A | 0.2287 | 0.0343 | 0.6720 | 0.124* | |
| H11B | 0.2091 | −0.0831 | 0.7599 | 0.124* | |
| H11C | 0.2546 | −0.1149 | 0.6679 | 0.124* | |
| C12 | 0.29860 (19) | −0.1216 (4) | 0.8871 (4) | 0.0941 (14) | |
| H12A | 0.3245 | −0.0896 | 0.9440 | 0.141* | |
| H12B | 0.3141 | −0.1915 | 0.8360 | 0.141* | |
| H12C | 0.2690 | −0.1613 | 0.9293 | 0.141* | |
| C13 | 0.36706 (10) | 0.2802 (3) | 0.8142 (3) | 0.0403 (6) | |
| H13A | 0.3447 | 0.3457 | 0.7788 | 0.048* | |
| C14 | 0.42028 (10) | 0.2630 (3) | 0.7657 (2) | 0.0344 (6) | |

| | | | | |
|---|---|---|---|---|
| C15 | 0.43582 (11) | 0.3420 (3) | 0.6666 (3) | 0.0390 (6) |
| H15A | 0.4126 | 0.4092 | 0.6367 | 0.047* |
| C16 | 0.48415 (11) | 0.3248 (3) | 0.6105 (3) | 0.0394 (7) |
| C17 | 0.51775 (11) | 0.2242 (3) | 0.6607 (3) | 0.0415 (7) |
| H17A | 0.5506 | 0.2102 | 0.6251 | 0.050* |
| C18 | 0.50481 (10) | 0.1442 (3) | 0.7606 (3) | 0.0378 (6) |
| C19 | 0.45548 (10) | 0.1634 (3) | 0.8132 (2) | 0.0351 (6) |
| C20 | 0.50008 (12) | 0.4134 (3) | 0.5021 (3) | 0.0501 (8) |
| C21 | 0.45576 (16) | 0.4140 (5) | 0.4080 (4) | 0.0873 (13) |
| H21A | 0.4237 | 0.4480 | 0.4440 | 0.131* |
| H21B | 0.4502 | 0.3205 | 0.3788 | 0.131* |
| H21C | 0.4655 | 0.4738 | 0.3423 | 0.131* |
| C22 | 0.50891 (19) | 0.5640 (4) | 0.5434 (4) | 0.0891 (14) |
| H22A | 0.4775 | 0.5980 | 0.5823 | 0.134* |
| H22B | 0.5168 | 0.6218 | 0.4751 | 0.134* |
| H22C | 0.5380 | 0.5669 | 0.5990 | 0.134* |
| C23 | 0.55002 (16) | 0.3593 (5) | 0.4403 (4) | 0.0898 (14) |
| H23A | 0.5787 | 0.3581 | 0.4969 | 0.135* |
| H23B | 0.5589 | 0.4197 | 0.3742 | 0.135* |
| H23C | 0.5439 | 0.2662 | 0.4109 | 0.135* |
| C24 | 0.54360 (11) | 0.0404 (3) | 0.8163 (3) | 0.0484 (7) |
| H24A | 0.5223 | −0.0311 | 0.8570 | 0.058* |
| C25 | 0.57752 (15) | −0.0359 (4) | 0.7233 (4) | 0.0720 (11) |
| H25A | 0.6009 | −0.0999 | 0.7635 | 0.108* |
| H25B | 0.5980 | 0.0310 | 0.6787 | 0.108* |
| H25C | 0.5550 | −0.0869 | 0.6692 | 0.108* |
| C26 | 0.57654 (11) | 0.1120 (3) | 0.9126 (3) | 0.0453 (7) |
| C27 | 0.61133 (12) | 0.2191 (4) | 0.8845 (3) | 0.0595 (9) |
| H27A | 0.6149 | 0.2469 | 0.8047 | 0.071* |
| C28 | 0.64090 (15) | 0.2858 (4) | 0.9719 (4) | 0.0753 (12) |
| H28A | 0.6639 | 0.3579 | 0.9511 | 0.090* |
| C29 | 0.63612 (18) | 0.2449 (5) | 1.0891 (4) | 0.0883 (14) |
| H29A | 0.6560 | 0.2889 | 1.1485 | 0.106* |
| C30 | 0.60198 (18) | 0.1388 (5) | 1.1194 (4) | 0.0839 (12) |
| H30A | 0.5987 | 0.1112 | 1.1993 | 0.101* |
| C31 | 0.57252 (13) | 0.0728 (4) | 1.0313 (3) | 0.0631 (9) |
| H31A | 0.5496 | 0.0007 | 1.0526 | 0.076* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0451 (11) | 0.0618 (13) | 0.0441 (12) | 0.0068 (10) | 0.0068 (10) | 0.0183 (11) |
| N1 | 0.0306 (11) | 0.0593 (15) | 0.0424 (14) | −0.0006 (11) | 0.0055 (11) | 0.0033 (13) |
| C1 | 0.0327 (14) | 0.0546 (17) | 0.0388 (16) | 0.0000 (13) | 0.0058 (12) | 0.0033 (15) |
| C2 | 0.0379 (16) | 0.0617 (18) | 0.0373 (16) | −0.0015 (13) | 0.0073 (13) | 0.0017 (15) |
| C3 | 0.0375 (16) | 0.079 (2) | 0.055 (2) | −0.0110 (15) | 0.0061 (16) | −0.0081 (19) |
| C4 | 0.0375 (17) | 0.083 (2) | 0.073 (2) | −0.0009 (17) | 0.0173 (18) | −0.004 (2) |
| C5 | 0.0496 (19) | 0.068 (2) | 0.062 (2) | 0.0047 (16) | 0.0191 (18) | −0.0052 (19) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.0430 (17) | 0.0568 (19) | 0.0468 (18) | −0.0007 (14) | 0.0076 (15) | −0.0001 (16) |
| C7 | 0.054 (2) | 0.058 (2) | 0.063 (2) | −0.0073 (16) | 0.0126 (17) | −0.0091 (18) |
| C8 | 0.088 (6) | 0.087 (5) | 0.105 (6) | −0.007 (4) | −0.039 (5) | 0.009 (5) |
| C9 | 0.103 (6) | 0.062 (4) | 0.117 (7) | 0.002 (4) | −0.016 (5) | −0.004 (5) |
| C7' | 0.054 (2) | 0.058 (2) | 0.063 (2) | −0.0073 (16) | 0.0126 (17) | −0.0091 (18) |
| C8' | 0.097 (7) | 0.107 (8) | 0.100 (7) | −0.017 (6) | −0.023 (6) | −0.001 (6) |
| C9' | 0.104 (7) | 0.076 (6) | 0.123 (8) | −0.008 (5) | 0.000 (7) | 0.017 (6) |
| C10 | 0.0483 (17) | 0.071 (2) | 0.0425 (17) | −0.0054 (15) | 0.0089 (16) | −0.0042 (18) |
| C11 | 0.078 (3) | 0.102 (3) | 0.067 (2) | −0.020 (2) | 0.001 (2) | −0.028 (2) |
| C12 | 0.129 (4) | 0.083 (3) | 0.070 (3) | 0.034 (3) | 0.023 (3) | −0.001 (3) |
| C13 | 0.0318 (14) | 0.0524 (16) | 0.0368 (15) | 0.0004 (12) | −0.0002 (13) | 0.0025 (15) |
| C14 | 0.0303 (14) | 0.0432 (14) | 0.0298 (13) | −0.0047 (11) | −0.0031 (11) | 0.0008 (13) |
| C15 | 0.0345 (15) | 0.0472 (15) | 0.0351 (15) | 0.0012 (12) | −0.0038 (13) | 0.0037 (14) |
| C16 | 0.0347 (15) | 0.0487 (16) | 0.0346 (15) | −0.0063 (12) | −0.0004 (13) | 0.0021 (13) |
| C17 | 0.0293 (14) | 0.0566 (17) | 0.0385 (15) | −0.0018 (12) | 0.0038 (12) | 0.0012 (15) |
| C18 | 0.0327 (15) | 0.0434 (15) | 0.0371 (16) | 0.0001 (11) | −0.0028 (12) | 0.0002 (14) |
| C19 | 0.0337 (14) | 0.0413 (14) | 0.0303 (14) | −0.0061 (11) | −0.0007 (12) | 0.0023 (13) |
| C20 | 0.0473 (18) | 0.062 (2) | 0.0412 (18) | −0.0058 (14) | 0.0078 (14) | 0.0118 (16) |
| C21 | 0.081 (3) | 0.131 (4) | 0.051 (2) | −0.006 (2) | −0.005 (2) | 0.026 (3) |
| C22 | 0.116 (4) | 0.070 (3) | 0.081 (3) | −0.027 (2) | 0.019 (3) | 0.021 (2) |
| C23 | 0.073 (3) | 0.116 (3) | 0.081 (3) | 0.012 (2) | 0.038 (2) | 0.038 (3) |
| C24 | 0.0387 (16) | 0.0498 (17) | 0.0567 (19) | 0.0062 (13) | 0.0012 (15) | 0.0023 (16) |
| C25 | 0.067 (2) | 0.077 (3) | 0.072 (2) | 0.024 (2) | −0.003 (2) | −0.007 (2) |
| C26 | 0.0308 (14) | 0.0571 (18) | 0.0479 (18) | 0.0103 (13) | 0.0022 (14) | 0.0090 (16) |
| C27 | 0.0482 (19) | 0.073 (2) | 0.057 (2) | 0.0023 (17) | −0.0059 (17) | 0.0125 (19) |
| C28 | 0.055 (2) | 0.080 (3) | 0.091 (3) | −0.0040 (18) | −0.025 (2) | 0.013 (2) |
| C29 | 0.082 (3) | 0.099 (3) | 0.084 (3) | 0.009 (3) | −0.044 (3) | 0.000 (3) |
| C30 | 0.089 (3) | 0.106 (3) | 0.057 (2) | 0.011 (3) | −0.021 (2) | 0.018 (2) |
| C31 | 0.057 (2) | 0.079 (2) | 0.054 (2) | 0.0035 (17) | −0.0029 (18) | 0.0169 (19) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C19 | 1.354 (3) | C13—H13A | 0.9300 |
| O1—H1 | 0.93 (4) | C14—C15 | 1.392 (4) |
| N1—C13 | 1.272 (4) | C14—C19 | 1.405 (4) |
| N1—C1 | 1.443 (3) | C15—C16 | 1.381 (4) |
| C1—C6 | 1.398 (4) | C15—H15A | 0.9300 |
| C1—C2 | 1.400 (4) | C16—C17 | 1.398 (4) |
| C2—C3 | 1.395 (4) | C16—C20 | 1.526 (4) |
| C2—C10 | 1.516 (4) | C17—C18 | 1.387 (4) |
| C3—C4 | 1.372 (5) | C17—H17A | 0.9300 |
| C3—H3A | 0.9300 | C18—C19 | 1.389 (4) |
| C4—C5 | 1.376 (5) | C18—C24 | 1.525 (4) |
| C4—H4A | 0.9300 | C20—C22 | 1.527 (5) |
| C5—C6 | 1.392 (4) | C20—C23 | 1.527 (5) |
| C5—H5A | 0.9300 | C20—C21 | 1.532 (5) |
| C6—C7 | 1.520 (5) | C21—H21A | 0.9600 |
| C7—C8 | 1.480 (7) | C21—H21B | 0.9600 |
| C7—C9 | 1.535 (7) | C21—H21C | 0.9600 |

| | | | |
|---|---|---|---|
| C7—H7A | 0.9800 | C22—H22A | 0.9600 |
| C8—H8A | 0.9600 | C22—H22B | 0.9600 |
| C8—H8B | 0.9600 | C22—H22C | 0.9600 |
| C8—H8C | 0.9600 | C23—H23A | 0.9600 |
| C9—H9A | 0.9600 | C23—H23B | 0.9600 |
| C9—H9B | 0.9600 | C23—H23C | 0.9600 |
| C9—H9C | 0.9600 | C24—C26 | 1.519 (5) |
| C8'—H8'A | 0.9600 | C24—C25 | 1.528 (5) |
| C8'—H8'B | 0.9600 | C24—H24A | 0.9800 |
| C8'—H8'C | 0.9600 | C25—H25A | 0.9600 |
| C9'—H9'A | 0.9600 | C25—H25B | 0.9600 |
| C9'—H9'B | 0.9600 | C25—H25C | 0.9600 |
| C9'—H9'C | 0.9600 | C26—C31 | 1.375 (5) |
| C10—C11 | 1.509 (5) | C26—C27 | 1.385 (4) |
| C10—C12 | 1.517 (5) | C27—C28 | 1.381 (5) |
| C10—H10A | 0.9800 | C27—H27A | 0.9300 |
| C11—H11A | 0.9600 | C28—C29 | 1.366 (6) |
| C11—H11B | 0.9600 | C28—H28A | 0.9300 |
| C11—H11C | 0.9600 | C29—C30 | 1.373 (6) |
| C12—H12A | 0.9600 | C29—H29A | 0.9300 |
| C12—H12B | 0.9600 | C30—C31 | 1.383 (6) |
| C12—H12C | 0.9600 | C30—H30A | 0.9300 |
| C13—C14 | 1.458 (4) | C31—H31A | 0.9300 |
| C19—O1—H1 | 108 (2) | C16—C15—H15A | 118.6 |
| C13—N1—C1 | 119.5 (2) | C14—C15—H15A | 118.6 |
| C6—C1—C2 | 122.3 (3) | C15—C16—C17 | 116.0 (3) |
| C6—C1—N1 | 120.6 (3) | C15—C16—C20 | 121.6 (3) |
| C2—C1—N1 | 117.0 (3) | C17—C16—C20 | 122.4 (2) |
| C3—C2—C1 | 117.5 (3) | C18—C17—C16 | 123.7 (3) |
| C3—C2—C10 | 120.6 (3) | C18—C17—H17A | 118.1 |
| C1—C2—C10 | 121.8 (2) | C16—C17—H17A | 118.1 |
| C4—C3—C2 | 121.2 (3) | C17—C18—C19 | 118.4 (2) |
| C4—C3—H3A | 119.4 | C17—C18—C24 | 122.1 (3) |
| C2—C3—H3A | 119.4 | C19—C18—C24 | 119.5 (3) |
| C3—C4—C5 | 120.1 (3) | O1—C19—C18 | 118.8 (2) |
| C3—C4—H4A | 120.0 | O1—C19—C14 | 121.2 (2) |
| C5—C4—H4A | 120.0 | C18—C19—C14 | 120.0 (2) |
| C4—C5—C6 | 121.6 (3) | C16—C20—C22 | 108.8 (3) |
| C4—C5—H5A | 119.2 | C16—C20—C23 | 112.7 (3) |
| C6—C5—H5A | 119.2 | C22—C20—C23 | 109.5 (3) |
| C5—C6—C1 | 117.3 (3) | C16—C20—C21 | 110.4 (3) |
| C5—C6—C7 | 120.6 (3) | C22—C20—C21 | 108.0 (3) |
| C1—C6—C7 | 122.1 (3) | C23—C20—C21 | 107.4 (3) |
| C8—C7—C6 | 111.5 (5) | C20—C21—H21A | 109.5 |
| C8—C7—C9 | 108.9 (7) | C20—C21—H21B | 109.5 |
| C6—C7—C9 | 113.9 (4) | H21A—C21—H21B | 109.5 |
| C8—C7—H7A | 107.4 | C20—C21—H21C | 109.5 |
| C6—C7—H7A | 107.4 | H21A—C21—H21C | 109.5 |
| C9—C7—H7A | 107.4 | H21B—C21—H21C | 109.5 |

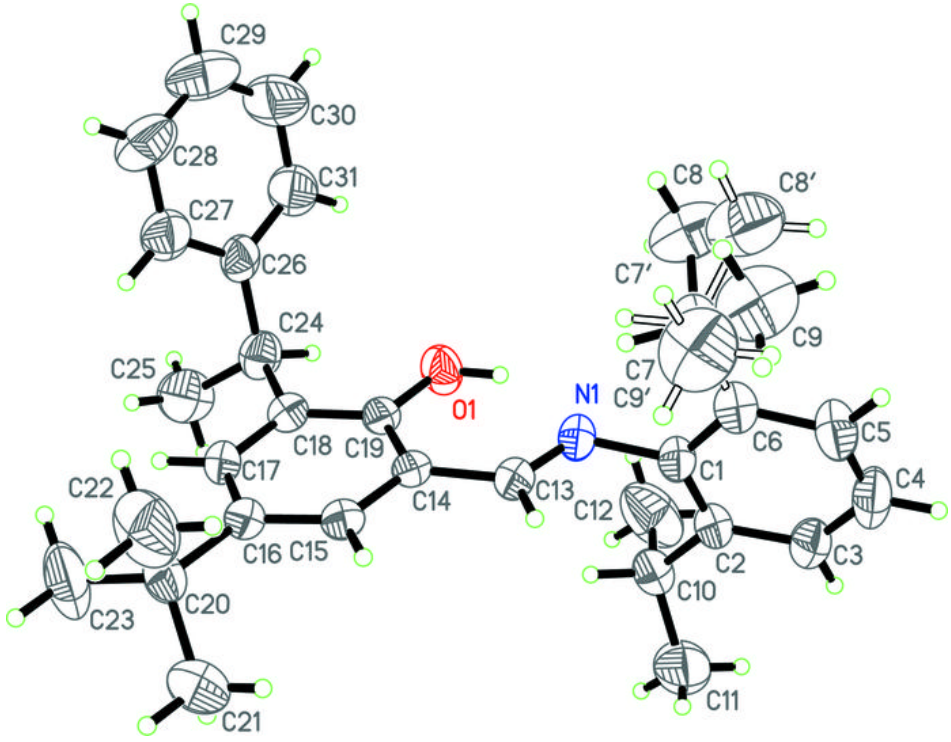
| | | | |
|---|---|---|---|
| C7—C8—H8A | 109.5 | C20—C22—H22A | 109.5 |
| C7—C8—H8B | 109.5 | C20—C22—H22B | 109.5 |
| H8A—C8—H8B | 109.5 | H22A—C22—H22B | 109.5 |
| C7—C8—H8C | 109.5 | C20—C22—H22C | 109.5 |
| H8A—C8—H8C | 109.5 | H22A—C22—H22C | 109.5 |
| H8B—C8—H8C | 109.5 | H22B—C22—H22C | 109.5 |
| C7—C9—H9A | 109.5 | C20—C23—H23A | 109.5 |
| C7—C9—H9B | 109.5 | C20—C23—H23B | 109.5 |
| H9A—C9—H9B | 109.5 | H23A—C23—H23B | 109.5 |
| C7—C9—H9C | 109.5 | C20—C23—H23C | 109.5 |
| H9A—C9—H9C | 109.5 | H23A—C23—H23C | 109.5 |
| H9B—C9—H9C | 109.5 | H23B—C23—H23C | 109.5 |
| H8'A—C8'—H8'B | 109.5 | C26—C24—C18 | 110.2 (2) |
| H8'A—C8'—H8'C | 109.5 | C26—C24—C25 | 112.6 (3) |
| H8'B—C8'—H8'C | 109.5 | C18—C24—C25 | 113.4 (3) |
| H9'A—C9'—H9'B | 109.5 | C26—C24—H24A | 106.7 |
| H9'A—C9'—H9'C | 109.5 | C18—C24—H24A | 106.7 |
| H9'B—C9'—H9'C | 109.5 | C25—C24—H24A | 106.7 |
| C11—C10—C2 | 113.6 (3) | C24—C25—H25A | 109.5 |
| C11—C10—C12 | 111.4 (3) | C24—C25—H25B | 109.5 |
| C2—C10—C12 | 109.3 (3) | H25A—C25—H25B | 109.5 |
| C11—C10—H10A | 107.4 | C24—C25—H25C | 109.5 |
| C2—C10—H10A | 107.4 | H25A—C25—H25C | 109.5 |
| C12—C10—H10A | 107.4 | H25B—C25—H25C | 109.5 |
| C10—C11—H11A | 109.5 | C31—C26—C27 | 117.7 (3) |
| C10—C11—H11B | 109.5 | C31—C26—C24 | 120.9 (3) |
| H11A—C11—H11B | 109.5 | C27—C26—C24 | 121.4 (3) |
| C10—C11—H11C | 109.5 | C28—C27—C26 | 121.7 (3) |
| H11A—C11—H11C | 109.5 | C28—C27—H27A | 119.1 |
| H11B—C11—H11C | 109.5 | C26—C27—H27A | 119.1 |
| C10—C12—H12A | 109.5 | C29—C28—C27 | 119.4 (4) |
| C10—C12—H12B | 109.5 | C29—C28—H28A | 120.3 |
| H12A—C12—H12B | 109.5 | C27—C28—H28A | 120.3 |
| C10—C12—H12C | 109.5 | C28—C29—C30 | 120.0 (4) |
| H12A—C12—H12C | 109.5 | C28—C29—H29A | 120.0 |
| H12B—C12—H12C | 109.5 | C30—C29—H29A | 120.0 |
| N1—C13—C14 | 122.7 (3) | C29—C30—C31 | 120.1 (4) |
| N1—C13—H13A | 118.6 | C29—C30—H30A | 120.0 |
| C14—C13—H13A | 118.6 | C31—C30—H30A | 120.0 |
| C15—C14—C19 | 119.0 (2) | C26—C31—C30 | 121.1 (4) |
| C15—C14—C13 | 119.5 (2) | C26—C31—H31A | 119.5 |
| C19—C14—C13 | 121.4 (2) | C30—C31—H31A | 119.5 |
| C16—C15—C14 | 122.9 (3) | | |
| C13—N1—C1—C6 | −87.7 (3) | C16—C17—C18—C19 | 0.9 (4) |
| C13—N1—C1—C2 | 96.7 (3) | C16—C17—C18—C24 | −177.1 (3) |
| C6—C1—C2—C3 | 0.5 (4) | C17—C18—C19—O1 | 179.0 (2) |
| N1—C1—C2—C3 | 176.1 (3) | C24—C18—C19—O1 | −3.0 (4) |
| C6—C1—C2—C10 | −176.7 (3) | C17—C18—C19—C14 | −0.7 (4) |
| N1—C1—C2—C10 | −1.2 (4) | C24—C18—C19—C14 | 177.3 (3) |

| | | | |
|---|---|---|---|
| C1—C2—C3—C4 | 0.4 (5) | C15—C14—C19—O1 | 179.9 (2) |
| C10—C2—C3—C4 | 177.8 (3) | C13—C14—C19—O1 | −3.3 (4) |
| C2—C3—C4—C5 | −0.1 (6) | C15—C14—C19—C18 | −0.4 (4) |
| C3—C4—C5—C6 | −1.3 (6) | C13—C14—C19—C18 | 176.4 (3) |
| C4—C5—C6—C1 | 2.2 (5) | C15—C16—C20—C22 | 69.1 (4) |
| C4—C5—C6—C7 | −175.8 (3) | C17—C16—C20—C22 | −109.4 (3) |
| C2—C1—C6—C5 | −1.8 (4) | C15—C16—C20—C23 | −169.3 (3) |
| N1—C1—C6—C5 | −177.2 (3) | C17—C16—C20—C23 | 12.2 (4) |
| C2—C1—C6—C7 | 176.2 (3) | C15—C16—C20—C21 | −49.2 (4) |
| N1—C1—C6—C7 | 0.8 (4) | C17—C16—C20—C21 | 132.3 (3) |
| C5—C6—C7—C8 | 94.5 (6) | C17—C18—C24—C26 | 90.3 (3) |
| C1—C6—C7—C8 | −83.4 (6) | C19—C18—C24—C26 | −87.6 (3) |
| C5—C6—C7—C9 | −29.2 (7) | C17—C18—C24—C25 | −37.0 (4) |
| C1—C6—C7—C9 | 152.9 (6) | C19—C18—C24—C25 | 145.1 (3) |
| C3—C2—C10—C11 | 36.4 (4) | C18—C24—C26—C31 | 115.0 (3) |
| C1—C2—C10—C11 | −146.4 (3) | C25—C24—C26—C31 | −117.3 (4) |
| C3—C2—C10—C12 | −88.6 (4) | C18—C24—C26—C27 | −64.6 (4) |
| C1—C2—C10—C12 | 88.6 (4) | C25—C24—C26—C27 | 63.1 (4) |
| C1—N1—C13—C14 | −172.8 (3) | C31—C26—C27—C28 | −0.5 (5) |
| N1—C13—C14—C15 | 178.5 (3) | C24—C26—C27—C28 | 179.2 (3) |
| N1—C13—C14—C19 | 1.7 (4) | C26—C27—C28—C29 | 0.4 (6) |
| C19—C14—C15—C16 | 1.4 (4) | C27—C28—C29—C30 | −0.3 (7) |
| C13—C14—C15—C16 | −175.5 (3) | C28—C29—C30—C31 | 0.2 (7) |
| C14—C15—C16—C17 | −1.2 (4) | C27—C26—C31—C30 | 0.4 (5) |
| C14—C15—C16—C20 | −179.8 (3) | C24—C26—C31—C30 | −179.2 (3) |
| C15—C16—C17—C18 | 0.1 (4) | C29—C30—C31—C26 | −0.3 (6) |
| C20—C16—C17—C18 | 178.7 (3) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N1 | 0.93 (4) | 1.79 (4) | 2.620 (3) | 147 (3) |

**Fig. 1**


C29
C30
C28
C31
C27
C26
C24
C25
C18
C19
O1
N1
C17
C22
C14
C13
C16
C15
C20
C23
C21
C8
C8′
C7′
C9
C7
C9′
C6
C5
C1
C4
C12
C2
C3
C10
C11