Acta Crystallographica Section E

**Structure Reports Online**

ISSN 1600-5368

# 2-Benzhydryl-6-*tert*-butyl-4-methylphenol

**Sungwoo Yoon,[a] Junseong Lee[b] and Youngjo Kim[a]***

[a]Department of Chemistry, Chungbuk National University, Cheongju, Chungbuk 361-763, Republic of Korea, and [b]Department of Chemistry, Chonnam National University, Gwangju 500-757, Republic of Korea
Correspondence e-mail: ykim@chungbuk.ac.kr

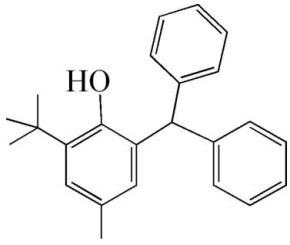
Received 28 November 2012; accepted 21 January 2013

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.071; $wR$ factor = 0.172; data-to-parameter ratio = 14.8.

The title compound, $C_{24}H_{26}O$, was prepared by the reaction between 2-*tert*-butyl-4-methylphenol and diphenylmethanol in the presence of sulfuric acid. Three benzene rings are attached directly to the central C—H group in a twisted propeller conformation with the local pseudo-$C_3$ rotational axis coinciding with the C—H bond. There are three short C—H···O contacts in the molecule.

## Related literature

For similar structure types, see: Kim *et al.* (2012).




## Experimental

### Crystal data

$C_{24}H_{26}O$ $M_r$ = 330.45
Monoclinic, $P2_1/n$
$a$ = 8.014 (4) Å
$b$ = 15.472 (7) Å
$c$ = 16.006 (7) Å
$\beta$ = 99.98 (2)°
$V$ = 1954.6 (15) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 296 K
0.20 × 0.17 × 0.15 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.987, $T_{max}$ = 0.990
17522 measured reflections
3422 independent reflections
1532 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.138

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.172
$S$ = 1.00
3422 reflections
231 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8*C*···O | 0.96 | 2.41 | 3.049 (4) | 123 |
| C10—H10*A*···O | 0.96 | 2.44 | 3.071 (5) | 123 |
| C12—H12···O | 0.98 | 2.38 | 2.771 (4) | 103 |

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

YK gratefully acknowledges financial support from the National Research Foundation of Korea (NRF) grant funded by the Korea government (MEST) (No. 2010–0007092).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2218).

## References

Bruker (2009). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Kim, S. H., Yoon, S., Mun, S.-D., Lee, H.-H., Lee, J. & Kim, Y. (2012). *Polyhedron*, **31**, 665–670.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2013). E**69**, o287 [doi:10.1107/S1600536813002006]

## 2-Benzhydryl-6-*tert*-butyl-4-methylphenol

**Sungwoo Yoon, Junseong Lee and Youngjo Kim**

### S1. Comment

The molecular structure of the title compound, $C_{24}H_{26}O$, is shown in Figure 1. The C—O and C—C bond lengths in the phenol ring and two phenyl rings are in the range of typical values determined on similar compounds (Kim *et al.* 2012). The three aromatic rings are twisted and form a propeller conformation with the local pseudo-$C_3$ rotational axis coinciding with C12—H12. The orientation of the rings can be characterized by the torsion angles H12-C12-C2-C1 (-35 °), H12-C12-C19-C24 (-59 °) and H12-C12-C13-C14 (-26 °). The molecules display three intramolecular C—H···O contacts (geometric details are given in Table 1), but no intermolecular hydrogen bonds are present.

### S2. Experimental

The title compound could be isolated in 94% yield *via* the reaction of sulfuric acid, 2-*tert*-butyl-4-methylphenol, and diphenylmethanol in glacial acetic acid. The crystal was obtained by slow evaporation of solvent in refrigerator.

### S3. Refinement

The H-atoms were included in calculated positions and treated as riding atoms with with C—H = 0.93–0.98 Å and O—H = 0.82 Å: $U_{iso}$(H) = 1.2 $U_{eq}$(parent C-atom),$U_{iso}$(H) = 1.5 $U_{eq}$(parent O-atom). The initial position of the hydroxyl H was derived from an electron density calculation.

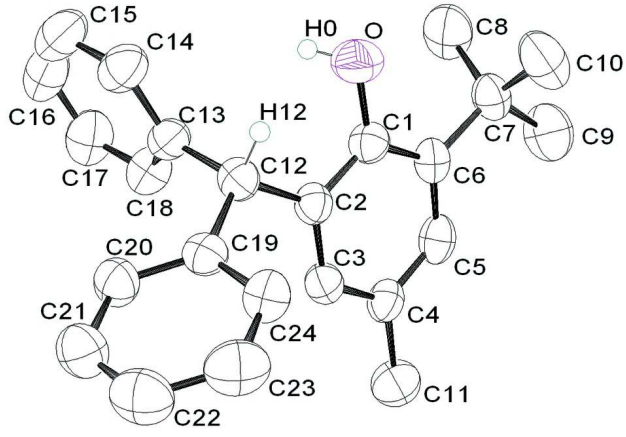



**Figure 1**

Molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms, with exception of H12 and H0, are omitted for clarity.

## 2-Benzhydryl-6-*tert*-butyl-4-methylphenol

*Crystal data*

$C_{24}H_{26}O$
$M_r = 330.45$
Monoclinic, $P2_1/n$
$a = 8.014$ (4) Å
$b = 15.472$ (7) Å
$c = 16.006$ (7) Å
$\beta = 99.98$ (2)°
$V = 1954.6$ (15) Å$^3$
$Z = 4$
$F(000) = 712$
$D_x = 1.123$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 925 reflections
$\theta = 2.7$–16.4°
$\mu = 0.07$ mm$^{-1}$
$T = 296$ K
Block, colorless
0.20 × 0.17 × 0.15 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.987$, $T_{max} = 0.990$
17522 measured reflections
3422 independent reflections
1532 reflections with $I > 2\sigma(I)$
$R_{int} = 0.138$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.6°$
$h = -9 \rightarrow 9$
$k = -17 \rightarrow 17$
$l = -18 \rightarrow 19$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.071$
$wR(F^2) = 0.172$
$S = 1.00$
3422 reflections
231 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0803P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å$^{-3}$
$\Delta\rho_{min} = -0.21$ e Å$^{-3}$

*Special details*

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

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$- factors based on ALL data will be even larger.

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O | −0.0324 (3) | 0.35794 (17) | 0.04276 (16) | 0.0721 (8) |
| H0 | −0.0789 | 0.3841 | 0.0769 | 0.108* |
| C3 | 0.3942 (4) | 0.3867 (2) | 0.1619 (2) | 0.0473 (9) |
| H3 | 0.4591 | 0.4304 | 0.1914 | 0.057* |
| C2 | 0.2285 (4) | 0.4048 (2) | 0.1234 (2) | 0.0436 (9) |

| | | | | |
|---|---|---|---|---|
| C13 | 0.0376 (4) | 0.4945 (2) | 0.1985 (2) | 0.0477 (9) |
| C1 | 0.1322 (4) | 0.3377 (2) | 0.0801 (2) | 0.0459 (9) |
| C5 | 0.3647 (5) | 0.2417 (2) | 0.1124 (2) | 0.0523 (10) |
| H5 | 0.4114 | 0.1871 | 0.1088 | 0.063* |
| C4 | 0.4652 (4) | 0.3057 (2) | 0.1578 (2) | 0.0480 (9) |
| C6 | 0.1977 (4) | 0.2555 (2) | 0.0721 (2) | 0.0473 (9) |
| C24 | 0.3685 (4) | 0.5791 (2) | 0.0708 (2) | 0.0551 (10) |
| H24 | 0.3627 | 0.5374 | 0.0285 | 0.066* |
| C19 | 0.2722 (4) | 0.5693 (2) | 0.1352 (2) | 0.0442 (9) |
| C12 | 0.1469 (4) | 0.4931 (2) | 0.1297 (2) | 0.0449 (9) |
| H12 | 0.0684 | 0.5009 | 0.0761 | 0.054* |
| C21 | 0.3905 (5) | 0.7026 (2) | 0.1965 (3) | 0.0645 (11) |
| H21 | 0.3976 | 0.7441 | 0.2389 | 0.077* |
| C23 | 0.4725 (5) | 0.6503 (3) | 0.0696 (3) | 0.0688 (12) |
| H23 | 0.5354 | 0.6564 | 0.0263 | 0.083* |
| C20 | 0.2870 (4) | 0.6314 (2) | 0.1981 (2) | 0.0535 (10) |
| H20 | 0.2263 | 0.6252 | 0.2422 | 0.064* |
| C14 | −0.1169 (5) | 0.5383 (2) | 0.1838 (3) | 0.0633 (11) |
| H14 | −0.1529 | 0.5650 | 0.1317 | 0.076* |
| C7 | 0.0933 (5) | 0.1835 (2) | 0.0202 (2) | 0.0565 (10) |
| C18 | 0.0871 (5) | 0.4564 (2) | 0.2772 (2) | 0.0593 (10) |
| H18 | 0.1895 | 0.4267 | 0.2882 | 0.071* |
| C17 | −0.0125 (6) | 0.4612 (3) | 0.3404 (3) | 0.0739 (12) |
| H17 | 0.0227 | 0.4351 | 0.3928 | 0.089* |
| C22 | 0.4836 (5) | 0.7122 (3) | 0.1319 (3) | 0.0708 (12) |
| H22 | 0.5530 | 0.7602 | 0.1306 | 0.085* |
| C8 | −0.0686 (5) | 0.1625 (2) | 0.0564 (3) | 0.0857 (14) |
| H8A | −0.0378 | 0.1443 | 0.1144 | 0.129* |
| H8B | −0.1298 | 0.1170 | 0.0238 | 0.129* |
| H8C | −0.1386 | 0.2131 | 0.0537 | 0.129* |
| C9 | 0.1948 (5) | 0.0992 (2) | 0.0221 (3) | 0.0924 (15) |
| H9A | 0.2963 | 0.1094 | −0.0006 | 0.139* |
| H9B | 0.1274 | 0.0562 | −0.0115 | 0.139* |
| H9C | 0.2240 | 0.0791 | 0.0795 | 0.139* |
| C15 | −0.2170 (5) | 0.5426 (3) | 0.2458 (3) | 0.0772 (13) |
| H15 | −0.3209 | 0.5708 | 0.2347 | 0.093* |
| C16 | −0.1636 (6) | 0.5053 (3) | 0.3238 (3) | 0.0807 (14) |
| H16 | −0.2302 | 0.5099 | 0.3657 | 0.097* |
| C10 | 0.0469 (6) | 0.2111 (3) | −0.0734 (2) | 0.0864 (14) |
| H10A | −0.0214 | 0.2624 | −0.0775 | 0.130* |
| H10B | −0.0155 | 0.1655 | −0.1056 | 0.130* |
| H10C | 0.1485 | 0.2225 | −0.0956 | 0.130* |
| C11 | 0.6475 (5) | 0.2879 (2) | 0.1987 (2) | 0.0733 (12) |
| H11A | 0.7193 | 0.2921 | 0.1567 | 0.110* |
| H11B | 0.6558 | 0.2308 | 0.2227 | 0.110* |
| H11C | 0.6828 | 0.3295 | 0.2427 | 0.110* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O | 0.0540 (17) | 0.071 (2) | 0.086 (2) | 0.0068 (14) | −0.0039 (15) | −0.0090 (16) |
| C3 | 0.049 (2) | 0.048 (2) | 0.044 (2) | 0.0002 (18) | 0.0064 (18) | −0.0042 (18) |
| C2 | 0.047 (2) | 0.040 (2) | 0.043 (2) | 0.0048 (18) | 0.0068 (17) | −0.0015 (18) |
| C13 | 0.044 (2) | 0.037 (2) | 0.064 (3) | −0.0031 (17) | 0.014 (2) | 0.0000 (19) |
| C1 | 0.047 (2) | 0.043 (2) | 0.047 (2) | 0.0051 (19) | 0.0068 (18) | 0.0031 (19) |
| C5 | 0.071 (3) | 0.037 (2) | 0.052 (2) | 0.009 (2) | 0.021 (2) | 0.0022 (19) |
| C4 | 0.051 (2) | 0.048 (2) | 0.046 (2) | 0.013 (2) | 0.0101 (18) | −0.0005 (19) |
| C6 | 0.060 (3) | 0.041 (2) | 0.044 (2) | 0.0000 (19) | 0.0153 (19) | −0.0031 (19) |
| C24 | 0.060 (2) | 0.053 (3) | 0.054 (2) | 0.003 (2) | 0.015 (2) | 0.000 (2) |
| C19 | 0.043 (2) | 0.040 (2) | 0.047 (2) | 0.0047 (17) | 0.0011 (18) | 0.0055 (19) |
| C12 | 0.049 (2) | 0.038 (2) | 0.047 (2) | 0.0041 (17) | 0.0030 (17) | 0.0017 (17) |
| C21 | 0.068 (3) | 0.048 (3) | 0.077 (3) | −0.005 (2) | 0.011 (2) | −0.005 (2) |
| C23 | 0.066 (3) | 0.072 (3) | 0.071 (3) | −0.013 (2) | 0.021 (2) | 0.019 (3) |
| C20 | 0.057 (2) | 0.045 (2) | 0.060 (2) | −0.0050 (19) | 0.0153 (19) | −0.004 (2) |
| C14 | 0.055 (2) | 0.051 (3) | 0.086 (3) | 0.003 (2) | 0.019 (2) | 0.003 (2) |
| C7 | 0.068 (3) | 0.047 (3) | 0.054 (3) | −0.007 (2) | 0.013 (2) | −0.009 (2) |
| C18 | 0.063 (2) | 0.055 (3) | 0.062 (3) | 0.006 (2) | 0.019 (2) | 0.008 (2) |
| C17 | 0.088 (3) | 0.062 (3) | 0.079 (3) | −0.004 (2) | 0.036 (3) | 0.005 (2) |
| C22 | 0.070 (3) | 0.056 (3) | 0.084 (3) | −0.012 (2) | 0.009 (3) | 0.009 (3) |
| C8 | 0.091 (3) | 0.071 (3) | 0.102 (3) | −0.032 (3) | 0.037 (3) | −0.019 (3) |
| C9 | 0.108 (4) | 0.047 (3) | 0.121 (4) | −0.003 (3) | 0.018 (3) | −0.027 (3) |
| C15 | 0.058 (3) | 0.063 (3) | 0.116 (4) | 0.008 (2) | 0.031 (3) | 0.001 (3) |
| C16 | 0.083 (3) | 0.059 (3) | 0.112 (4) | 0.001 (3) | 0.050 (3) | −0.006 (3) |
| C10 | 0.104 (4) | 0.089 (3) | 0.063 (3) | −0.025 (3) | 0.009 (3) | −0.018 (3) |
| C11 | 0.059 (3) | 0.075 (3) | 0.081 (3) | 0.018 (2) | 0.000 (2) | −0.002 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O—C1 | 1.386 (4) | C20—H20 | 0.9300 |
| O—H0 | 0.8200 | C14—C15 | 1.382 (5) |
| C3—C4 | 1.382 (4) | C14—H14 | 0.9300 |
| C3—C2 | 1.392 (4) | C7—C9 | 1.535 (5) |
| C3—H3 | 0.9300 | C7—C10 | 1.541 (5) |
| C2—C1 | 1.403 (4) | C7—C8 | 1.545 (5) |
| C2—C12 | 1.526 (4) | C18—C17 | 1.395 (5) |
| C13—C18 | 1.386 (4) | C18—H18 | 0.9300 |
| C13—C14 | 1.395 (4) | C17—C16 | 1.375 (5) |
| C13—C12 | 1.521 (4) | C17—H17 | 0.9300 |
| C1—C6 | 1.390 (4) | C22—H22 | 0.9300 |
| C5—C6 | 1.398 (4) | C8—H8A | 0.9600 |
| C5—C4 | 1.398 (5) | C8—H8B | 0.9600 |
| C5—H5 | 0.9300 | C8—H8C | 0.9600 |
| C4—C11 | 1.519 (5) | C9—H9A | 0.9600 |
| C6—C7 | 1.546 (5) | C9—H9B | 0.9600 |
| C24—C23 | 1.384 (5) | C9—H9C | 0.9600 |

| | | | |
|---|---|---|---|
| C24—C19 | 1.400 (4) | C15—C16 | 1.374 (5) |
| C24—H24 | 0.9300 | C15—H15 | 0.9300 |
| C19—C20 | 1.382 (4) | C16—H16 | 0.9300 |
| C19—C12 | 1.540 (4) | C10—H10A | 0.9600 |
| C12—H12 | 0.9800 | C10—H10B | 0.9600 |
| C21—C20 | 1.381 (5) | C10—H10C | 0.9600 |
| C21—C22 | 1.384 (5) | C11—H11A | 0.9600 |
| C21—H21 | 0.9300 | C11—H11B | 0.9600 |
| C23—C22 | 1.373 (5) | C11—H11C | 0.9600 |
| C23—H23 | 0.9300 | | |

| | | | |
|---|---|---|---|
| C1—O—H0 | 109.5 | C9—C7—C10 | 107.0 (3) |
| C4—C3—C2 | 122.0 (3) | C9—C7—C8 | 106.9 (3) |
| C4—C3—H3 | 119.0 | C10—C7—C8 | 110.3 (3) |
| C2—C3—H3 | 119.0 | C9—C7—C6 | 111.5 (3) |
| C3—C2—C1 | 118.1 (3) | C10—C7—C6 | 109.9 (3) |
| C3—C2—C12 | 122.5 (3) | C8—C7—C6 | 111.2 (3) |
| C1—C2—C12 | 119.3 (3) | C13—C18—C17 | 121.8 (4) |
| C18—C13—C14 | 117.8 (3) | C13—C18—H18 | 119.1 |
| C18—C13—C12 | 122.8 (3) | C17—C18—H18 | 119.1 |
| C14—C13—C12 | 119.4 (3) | C16—C17—C18 | 118.8 (4) |
| O—C1—C6 | 120.9 (3) | C16—C17—H17 | 120.6 |
| O—C1—C2 | 116.5 (3) | C18—C17—H17 | 120.6 |
| C6—C1—C2 | 122.6 (3) | C23—C22—C21 | 119.4 (4) |
| C6—C5—C4 | 123.4 (3) | C23—C22—H22 | 120.3 |
| C6—C5—H5 | 118.3 | C21—C22—H22 | 120.3 |
| C4—C5—H5 | 118.3 | C7—C8—H8A | 109.5 |
| C3—C4—C5 | 117.5 (3) | C7—C8—H8B | 109.5 |
| C3—C4—C11 | 121.1 (3) | H8A—C8—H8B | 109.5 |
| C5—C4—C11 | 121.3 (3) | C7—C8—H8C | 109.5 |
| C1—C6—C5 | 116.4 (3) | H8A—C8—H8C | 109.5 |
| C1—C6—C7 | 122.1 (3) | H8B—C8—H8C | 109.5 |
| C5—C6—C7 | 121.6 (3) | C7—C9—H9A | 109.5 |
| C23—C24—C19 | 120.4 (4) | C7—C9—H9B | 109.5 |
| C23—C24—H24 | 119.8 | H9A—C9—H9B | 109.5 |
| C19—C24—H24 | 119.8 | C7—C9—H9C | 109.5 |
| C20—C19—C24 | 118.2 (3) | H9A—C9—H9C | 109.5 |
| C20—C19—C12 | 123.2 (3) | H9B—C9—H9C | 109.5 |
| C24—C19—C12 | 118.5 (3) | C16—C15—C14 | 120.3 (4) |
| C13—C12—C2 | 111.6 (3) | C16—C15—H15 | 119.8 |
| C13—C12—C19 | 113.5 (3) | C14—C15—H15 | 119.8 |
| C2—C12—C19 | 114.0 (3) | C15—C16—C17 | 120.6 (4) |
| C13—C12—H12 | 105.6 | C15—C16—H16 | 119.7 |
| C2—C12—H12 | 105.6 | C17—C16—H16 | 119.7 |
| C19—C12—H12 | 105.6 | C7—C10—H10A | 109.5 |
| C20—C21—C22 | 120.2 (4) | C7—C10—H10B | 109.5 |
| C20—C21—H21 | 119.9 | H10A—C10—H10B | 109.5 |
| C22—C21—H21 | 119.9 | C7—C10—H10C | 109.5 |

| | | | |
|---|---|---|---|
| C22—C23—C24 | 120.6 (4) | H10A—C10—H10C | 109.5 |
| C22—C23—H23 | 119.7 | H10B—C10—H10C | 109.5 |
| C24—C23—H23 | 119.7 | C4—C11—H11A | 109.5 |
| C21—C20—C19 | 121.2 (4) | C4—C11—H11B | 109.5 |
| C21—C20—H20 | 119.4 | H11A—C11—H11B | 109.5 |
| C19—C20—H20 | 119.4 | C4—C11—H11C | 109.5 |
| C15—C14—C13 | 120.7 (4) | H11A—C11—H11C | 109.5 |
| C15—C14—H14 | 119.6 | H11B—C11—H11C | 109.5 |
| C13—C14—H14 | 119.6 | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8*C*···O | 0.96 | 2.41 | 3.049 (4) | 123 |
| C10—H10*A*···O | 0.96 | 2.44 | 3.071 (5) | 123 |
| C12—H12···O | 0.98 | 2.38 | 2.771 (4) | 103 |