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# 4-Benzyloxy-1-oxaspiro[4.6]undec-3-en-2-one

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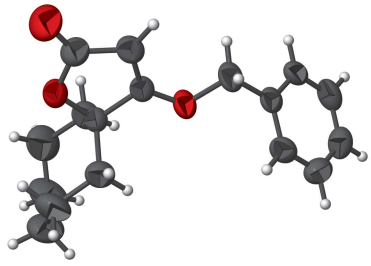
**CCDC reference**: 1507508

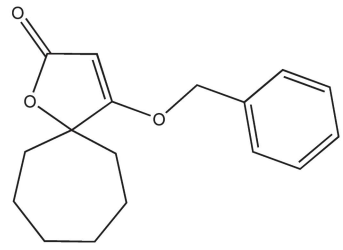
**Structural data**: full structural data are available from iucrdata.iucr.org

The title compound, $C_{17}H_{20}O_3$, the cycloheptane ring adopts a slightly distorted chair conformation. The planar five-membered ring is inclined at 57.13 (11)° to the phenyl ring of the benzyloxy substituent. In the crystal structure, C—H···O and C—H···$\pi$ hydrogen bonds generate layers in the *ac* plane.

**3D view**



**Chemical scheme**



## Structure description

The 4-hydroxyfuran-2[5*H*]-one core ($\beta$-tetronic acid) is present in diverse compounds isolated from natural products. These compounds have shown a variety of biological activities (Schobert & Schlenk, 2008). The synthesis and structural analysis of related derivatives continues to be of significant interest. Although several methodologies have been reported for their preparation, most of them use expensive organic starting materials as the synthesis is complex (Tejedor & García-Tellado, 2004). $\alpha$-Hydroxyesters and their cycloalkane derivatives can be easily prepared and then used for the direct synthesis of butenolides (furan-2[5*H*]-ones) through an addition followed by a Wittig olefination reaction using the accumulated ylide $Ph_3P{=}C{=}C{=}O$; the use of cycloalkane-$\alpha$-hydroxyesters allows the preparation of spiro systems of analogous substances with antiviral and anticancer activities among their most important properties (Schobert, 2007).

In the title compound (Fig. 1), the cycloheptane ring adopts a slightly distorted chair conformation with $q2$ = 0.438 (3) Å and $\varphi$ = 20.8 (4)°. The orientation of the five-membered ring (O1/C1/C4/C3/C2) with respect to the cycloheptane ring is similar to that reported by Schobert *et al.* (2001) for spiro-compounds with seven membered rings. The mean plane of the five-membered ring forms a dihedral angle of 57.13 (11)° with the phenyl ring of the benzyloxy substituent. In the molecule there is a very weak C9—H9*B*···O1 contact present (Table 1).

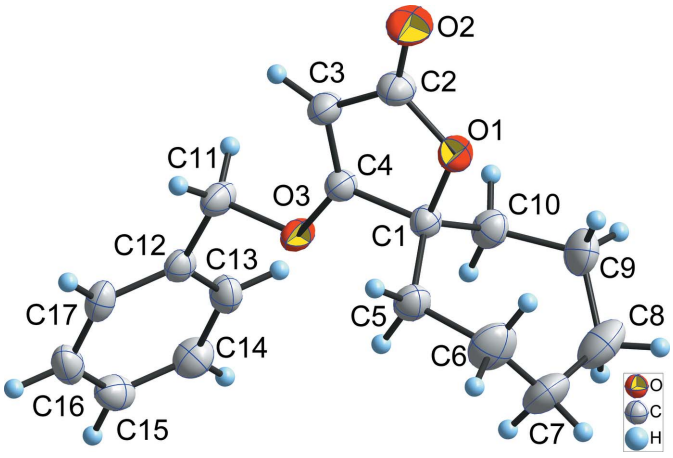



**Figure 1**
View of the title compound with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

In the crystal, molecules are connected by C16—H16···O2 contacts, generating zigzag *C*(10) chains parallel to the *c* axis (Fig. 2). C7—H7*B*···$\pi$ interactions form between the cycloheptane ring and the centroid *Cg*2 of the benzene ring. These contacts link the molecules into dimers, forming inversion dimers (Fig. 3), and creating double chains of molecules approximately along [01$\bar{1}$]. These double chains, shown in orange and green in Fig. 4, are further arranged back-to-back forming a layer structure.

The PDF-4/Organics (ICDD, 2012) and the Cambridge Structural Database (CSD) (Groom *et al.* 2016) both confirm that this is the first report of the structure of this material.

## Synthesis and crystallization

In a 250 ml Schlenk round-bottom flask under an argon atmosphere, 2.18 g (7.21 mmol) of keteneylidenetriphenylphosphorane ($Ph_3P$=C=C=O) and 150 ml of anhydrous

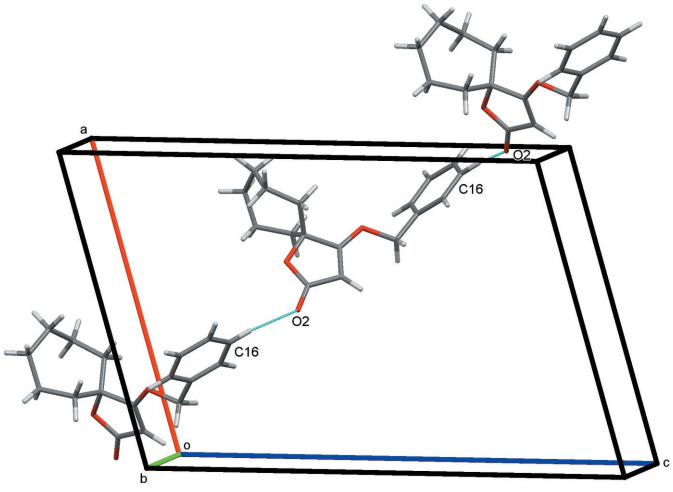



**Figure 2**
A view of the C—H···O hydrogen-bonded chain in the crystal structure of the title compound (see Table 1).

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

*Cg*2 is the centroid of the benzene ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C9—H9*B*···O1 | 0.97 | 2.56 | 2.987 (3) | 106 |
| C16—H16···O2$^{i}$ | 0.93 | 2.53 | 3.362 (3) | 149 |
| C7—H7*B*···*Cg*2$^{ii}$ | 0.97 | 2.80 | 3.750 (3) | 165 |

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x+2, -y+1, -z+1$.

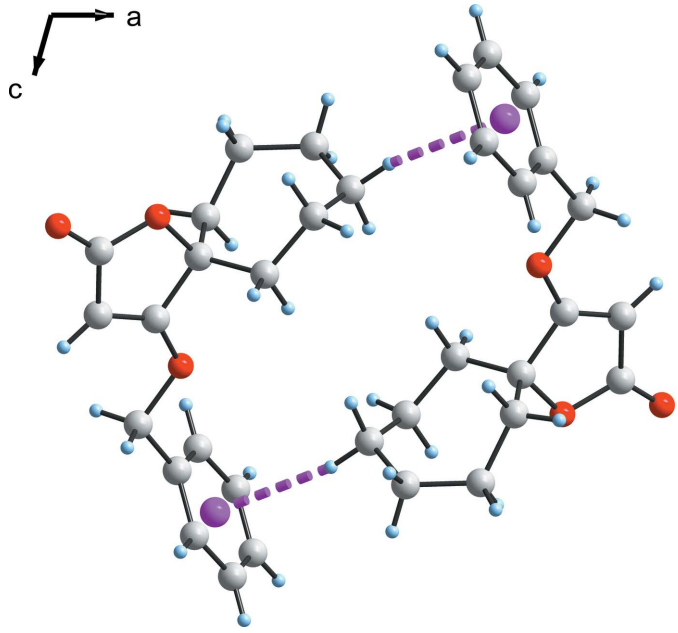



**Figure 3**
Inversion dimers formed by C—H···$\pi$ interactions.

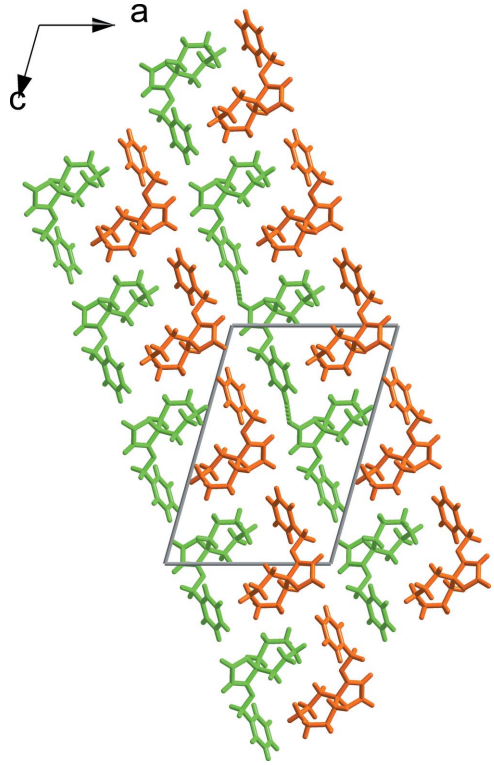



**Figure 4**
A view along the *b* axis showing the separate zigzag chains.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{17}H_{20}O_3$ |
| $M_r$ | 272.33 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 298 |
| $a, b, c$ (Å) | 13.1661 (9), 5.9457 (4), 19.6730 (13) |
| $\beta$ (°) | 105.774 (3) |
| $V$ (Å$^3$) | 1482.04 (17) |
| $Z$ | 4 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.66 |
| Crystal size (mm) | 0.26 × 0.17 × 0.08 |
| | |
| Data collection | |
| Diffractometer | Rigaku Pilatus 200K |
| Absorption correction | Analytical (Alcock, 1974) |
| $T_{min}$, $T_{max}$ | 0.653, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 10788, 2663, 1961 |
| $R_{int}$ | 0.028 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.601 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.047, 0.159, 1.12 |
| No. of reflections | 2663 |
| No. of parameters | 182 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.43, −0.19 |

Computer programs: *CrystalClear-SM Expert* (Rigaku, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *PLATON* (Spek, 2009).

toluene (freshly distilled over sodium) were added and stirred magnetically. 0.87 g (3.50 mmol) of benzyl-1-hydroxycycloheptanecarboxylate, previously dried under vacuum for 1 h, were then added. The reaction mixture was heated under reflux for 72 h (completion of the reaction was monitored by thin-layer chromatography). Toluene was removed by rotary evaporation. Triphenylphosphine oxide (TPPO) formed during the reaction was removed by dissolving the reaction residue in methylene chloride and then filtering it through a small column of silica gel (60 to 120 mesh). The methylene chloride was removed by rotary evaporation and the residual crude product was purified by column chromatography using silica gel (60 to 120 mesh) and hexane–ethyl acetate (5:1) as eluents to afford the pure title compound (yield 70%). $R_f = 0.4$ ($SiO_2$, hexane:ethyl acetate, 5:2). Colourless plate-shaped crystals were grown by slow evaporation in air at room temperature from a 1:1 ethyl acetate:ethanol solution [61% yield, m.p. 368 K].

## Refinement

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

## Acknowledgements

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# full crystallographic data

*IUCrData* (2016). **1**, x161538 [https://doi.org/10.1107/S2414314616015388]

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*Crystal data*

$C_{17}H_{20}O_3$
$M_r$ = 272.33
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 13.1661 (9) Å
$b$ = 5.9457 (4) Å
$c$ = 19.6730 (13) Å
$\beta$ = 105.774 (3)°
$V$ = 1482.04 (17) Å$^3$
$Z$ = 4
$F(000)$ = 584
$D_x$ = 1.220 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54187 Å
Cell parameters from 75 reflections
$\theta$ = 6.6–68.3°
$\mu$ = 0.66 mm$^{-1}$
$T$ = 298 K
Plate, colorless
0.26 × 0.17 × 0.08 mm

*Data collection*

Rigaku Pilatus 200K diffractometer
Confocal monochromator
Detector resolution: 5.8140 pixels mm$^{-1}$
profile data from $\omega$–scans
Absorption correction: analytical (Alcock, 1974)
$T_{min}$ = 0.653, $T_{max}$ = 1.000
10788 measured reflections
2663 independent reflections
1961 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 68.0°, $\theta_{min}$ = 7.0°
$h$ = −15→14
$k$ = −7→6
$l$ = −23→23

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.159
$S$ = 1.12
2663 reflections
182 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
W = 1/[$\Sigma^2$($FO^2$) + (0.0944$P$)$^2$ + 0.0383$P$] WHERE $P$ = ($FO^2$ + 2$FC^2$)/3
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$
Extinction correction: shelxl-2014/7 (Sheldrick 2015a, FC$^*$=KFC[1+0.001XFC$^2\Lambda^3$/SIN(2$\Theta$)]$^{-1/4}$
Extinction coefficient: 0.0055 (12)

*Special details*

**Geometry**. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.65557 (10) | 0.7811 (2) | 0.39735 (6) | 0.0587 (4) |
| O2 | 0.51051 (14) | 0.9560 (3) | 0.40696 (9) | 0.0926 (7) |
| O3 | 0.75329 (9) | 0.4593 (2) | 0.55237 (6) | 0.0586 (4) |
| C1 | 0.73395 (13) | 0.6282 (3) | 0.43863 (9) | 0.0466 (5) |
| C2 | 0.58293 (15) | 0.8307 (3) | 0.43300 (11) | 0.0616 (7) |
| C3 | 0.60803 (14) | 0.7127 (3) | 0.49933 (10) | 0.0572 (6) |
| C4 | 0.69565 (13) | 0.5954 (3) | 0.50349 (9) | 0.0483 (5) |
| C5 | 0.84009 (14) | 0.7456 (4) | 0.45714 (10) | 0.0615 (7) |
| C6 | 0.8889 (2) | 0.7882 (5) | 0.39683 (17) | 0.0958 (11) |
| C7 | 0.9329 (2) | 0.5925 (6) | 0.36911 (17) | 0.1085 (13) |
| C8 | 0.8603 (3) | 0.4293 (5) | 0.32391 (18) | 0.1036 (12) |
| C9 | 0.7490 (2) | 0.4241 (5) | 0.32610 (13) | 0.0845 (9) |
| C10 | 0.72762 (17) | 0.4081 (3) | 0.39760 (11) | 0.0616 (7) |
| C11 | 0.71428 (15) | 0.4155 (4) | 0.61342 (10) | 0.0626 (7) |
| C12 | 0.79198 (13) | 0.2632 (3) | 0.66139 (9) | 0.0481 (5) |
| C13 | 0.81346 (15) | 0.0543 (3) | 0.63809 (10) | 0.0573 (6) |
| C14 | 0.88756 (17) | −0.0856 (3) | 0.68052 (12) | 0.0673 (7) |
| C15 | 0.94012 (16) | −0.0186 (4) | 0.74684 (12) | 0.0668 (7) |
| C16 | 0.91935 (16) | 0.1878 (4) | 0.77136 (10) | 0.0647 (7) |
| C17 | 0.84535 (15) | 0.3281 (3) | 0.72885 (9) | 0.0555 (6) |
| H3 | 0.57020 | 0.71750 | 0.53290 | 0.0690* |
| H5A | 0.88920 | 0.65620 | 0.49250 | 0.0740* |
| H5B | 0.83240 | 0.88920 | 0.47860 | 0.0740* |
| H6A | 0.83550 | 0.85530 | 0.35820 | 0.1150* |
| H6B | 0.94480 | 0.89810 | 0.41250 | 0.1150* |
| H7A | 0.97630 | 0.51050 | 0.40920 | 0.1300* |
| H7B | 0.97960 | 0.64850 | 0.34240 | 0.1300* |
| H8A | 0.88950 | 0.28020 | 0.33610 | 0.1240* |
| H8B | 0.86070 | 0.45740 | 0.27540 | 0.1240* |
| H9A | 0.71510 | 0.29710 | 0.29810 | 0.1010* |
| H9B | 0.71490 | 0.55910 | 0.30310 | 0.1010* |
| H10A | 0.77770 | 0.30310 | 0.42630 | 0.0740* |
| H10B | 0.65770 | 0.34520 | 0.39110 | 0.0740* |
| H11A | 0.64540 | 0.34440 | 0.59890 | 0.0750* |
| H11B | 0.70780 | 0.55500 | 0.63740 | 0.0750* |
| H13 | 0.77730 | 0.00710 | 0.59290 | 0.0690* |
| H14 | 0.90160 | −0.22540 | 0.66390 | 0.0810* |
| H15 | 0.99020 | −0.11260 | 0.77560 | 0.0800* |
| H16 | 0.95530 | 0.23310 | 0.81680 | 0.0780* |

| | | | | |
|---|---|---|---|---|
| H17 | 0.83140 | 0.46740 | 0.74580 | 0.0670* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0626 (8) | 0.0623 (8) | 0.0523 (7) | 0.0119 (6) | 0.0175 (6) | 0.0119 (6) |
| O2 | 0.0841 (11) | 0.1050 (13) | 0.0885 (11) | 0.0474 (10) | 0.0234 (9) | 0.0288 (10) |
| O3 | 0.0541 (7) | 0.0765 (9) | 0.0513 (7) | 0.0182 (6) | 0.0248 (6) | 0.0183 (6) |
| C1 | 0.0483 (9) | 0.0480 (10) | 0.0446 (9) | 0.0035 (7) | 0.0146 (7) | 0.0037 (7) |
| C2 | 0.0574 (11) | 0.0630 (12) | 0.0641 (12) | 0.0134 (10) | 0.0159 (9) | 0.0070 (10) |
| C3 | 0.0516 (10) | 0.0673 (13) | 0.0567 (10) | 0.0096 (9) | 0.0215 (8) | 0.0037 (9) |
| C4 | 0.0460 (9) | 0.0526 (10) | 0.0478 (9) | 0.0035 (7) | 0.0154 (7) | 0.0037 (8) |
| C5 | 0.0572 (11) | 0.0668 (12) | 0.0639 (11) | −0.0080 (9) | 0.0223 (9) | −0.0029 (10) |
| C6 | 0.0947 (18) | 0.0952 (19) | 0.112 (2) | −0.0267 (15) | 0.0528 (16) | 0.0020 (16) |
| C7 | 0.0777 (16) | 0.158 (3) | 0.108 (2) | 0.0046 (18) | 0.0564 (16) | −0.013 (2) |
| C8 | 0.113 (2) | 0.102 (2) | 0.120 (2) | 0.0209 (18) | 0.0730 (19) | −0.0032 (18) |
| C9 | 0.0960 (17) | 0.0951 (17) | 0.0661 (14) | 0.0017 (14) | 0.0285 (12) | −0.0249 (12) |
| C10 | 0.0660 (12) | 0.0567 (12) | 0.0653 (12) | −0.0034 (9) | 0.0233 (9) | −0.0069 (9) |
| C11 | 0.0586 (11) | 0.0801 (14) | 0.0582 (11) | 0.0134 (10) | 0.0316 (9) | 0.0172 (10) |
| C12 | 0.0488 (9) | 0.0545 (10) | 0.0464 (9) | −0.0010 (8) | 0.0223 (7) | 0.0063 (8) |
| C13 | 0.0629 (11) | 0.0596 (12) | 0.0493 (10) | −0.0065 (9) | 0.0152 (8) | −0.0085 (9) |
| C14 | 0.0763 (13) | 0.0526 (11) | 0.0777 (14) | 0.0053 (10) | 0.0291 (11) | 0.0011 (10) |
| C15 | 0.0568 (11) | 0.0761 (14) | 0.0664 (13) | 0.0054 (10) | 0.0150 (10) | 0.0205 (11) |
| C16 | 0.0640 (12) | 0.0853 (15) | 0.0430 (9) | −0.0158 (11) | 0.0115 (8) | 0.0021 (10) |
| C17 | 0.0721 (12) | 0.0531 (10) | 0.0494 (10) | −0.0067 (9) | 0.0303 (9) | −0.0041 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.448 (2) | C16—C17 | 1.379 (3) |
| O1—C2 | 1.363 (2) | C3—H3 | 0.9300 |
| O2—C2 | 1.209 (3) | C5—H5A | 0.9700 |
| O3—C4 | 1.326 (2) | C5—H5B | 0.9700 |
| O3—C11 | 1.452 (2) | C6—H6A | 0.9700 |
| C1—C4 | 1.507 (2) | C6—H6B | 0.9700 |
| C1—C5 | 1.515 (3) | C7—H7A | 0.9700 |
| C1—C10 | 1.528 (3) | C7—H7B | 0.9700 |
| C2—C3 | 1.439 (3) | C8—H8A | 0.9700 |
| C3—C4 | 1.331 (3) | C8—H8B | 0.9700 |
| C5—C6 | 1.516 (4) | C9—H9A | 0.9700 |
| C6—C7 | 1.469 (4) | C9—H9B | 0.9700 |
| C7—C8 | 1.478 (5) | C10—H10A | 0.9700 |
| C8—C9 | 1.478 (5) | C10—H10B | 0.9700 |
| C9—C10 | 1.511 (3) | C11—H11A | 0.9700 |
| C11—C12 | 1.494 (3) | C11—H11B | 0.9700 |
| C12—C13 | 1.380 (3) | C13—H13 | 0.9300 |
| C12—C17 | 1.377 (2) | C14—H14 | 0.9300 |
| C13—C14 | 1.378 (3) | C15—H15 | 0.9300 |
| C14—C15 | 1.360 (3) | C16—H16 | 0.9300 |

| | | | |
|---|---|---|---|
| C15—C16 | 1.373 (3) | C17—H17 | 0.9300 |
| | | | |
| C1—O1—C2 | 109.88 (13) | C7—C6—H6A | 108.00 |
| C4—O3—C11 | 116.60 (14) | C7—C6—H6B | 108.00 |
| O1—C1—C4 | 101.81 (14) | H6A—C6—H6B | 107.00 |
| O1—C1—C5 | 108.41 (15) | C6—C7—H7A | 108.00 |
| O1—C1—C10 | 108.26 (14) | C6—C7—H7B | 108.00 |
| C4—C1—C5 | 110.81 (15) | C8—C7—H7A | 108.00 |
| C4—C1—C10 | 110.72 (15) | C8—C7—H7B | 108.00 |
| C5—C1—C10 | 115.84 (16) | H7A—C7—H7B | 107.00 |
| O1—C2—O2 | 119.88 (19) | C7—C8—H8A | 108.00 |
| O1—C2—C3 | 109.93 (16) | C7—C8—H8B | 108.00 |
| O2—C2—C3 | 130.2 (2) | C9—C8—H8A | 108.00 |
| C2—C3—C4 | 107.02 (17) | C9—C8—H8B | 108.00 |
| O3—C4—C1 | 115.83 (15) | H8A—C8—H8B | 107.00 |
| O3—C4—C3 | 132.82 (17) | C8—C9—H9A | 108.00 |
| C1—C4—C3 | 111.35 (16) | C8—C9—H9B | 108.00 |
| C1—C5—C6 | 116.63 (18) | C10—C9—H9A | 108.00 |
| C5—C6—C7 | 116.9 (3) | C10—C9—H9B | 108.00 |
| C6—C7—C8 | 119.2 (3) | H9A—C9—H9B | 107.00 |
| C7—C8—C9 | 118.7 (3) | C1—C10—H10A | 108.00 |
| C8—C9—C10 | 117.8 (2) | C1—C10—H10B | 108.00 |
| C1—C10—C9 | 116.15 (18) | C9—C10—H10A | 108.00 |
| O3—C11—C12 | 107.20 (15) | C9—C10—H10B | 108.00 |
| C11—C12—C13 | 120.19 (16) | H10A—C10—H10B | 107.00 |
| C11—C12—C17 | 121.41 (17) | O3—C11—H11A | 110.00 |
| C13—C12—C17 | 118.39 (17) | O3—C11—H11B | 110.00 |
| C12—C13—C14 | 121.18 (18) | C12—C11—H11A | 110.00 |
| C13—C14—C15 | 119.76 (19) | C12—C11—H11B | 110.00 |
| C14—C15—C16 | 120.1 (2) | H11A—C11—H11B | 108.00 |
| C15—C16—C17 | 120.20 (18) | C12—C13—H13 | 119.00 |
| C12—C17—C16 | 120.41 (17) | C14—C13—H13 | 119.00 |
| C2—C3—H3 | 126.00 | C13—C14—H14 | 120.00 |
| C4—C3—H3 | 127.00 | C15—C14—H14 | 120.00 |
| C1—C5—H5A | 108.00 | C14—C15—H15 | 120.00 |
| C1—C5—H5B | 108.00 | C16—C15—H15 | 120.00 |
| C6—C5—H5A | 108.00 | C15—C16—H16 | 120.00 |
| C6—C5—H5B | 108.00 | C17—C16—H16 | 120.00 |
| H5A—C5—H5B | 107.00 | C12—C17—H17 | 120.00 |
| C5—C6—H6A | 108.00 | C16—C17—H17 | 120.00 |
| C5—C6—H6B | 108.00 | | |
| | | | |
| C2—O1—C1—C4 | 0.28 (18) | O1—C2—C3—C4 | 0.6 (2) |
| C2—O1—C1—C5 | −116.60 (16) | O2—C2—C3—C4 | 179.7 (2) |
| C2—O1—C1—C10 | 117.00 (16) | C2—C3—C4—O3 | 179.77 (19) |
| C1—O1—C2—O2 | −179.77 (18) | C2—C3—C4—C1 | −0.4 (2) |
| C1—O1—C2—C3 | −0.6 (2) | C1—C5—C6—C7 | −73.6 (3) |
| C11—O3—C4—C1 | −176.58 (15) | C5—C6—C7—C8 | 75.0 (4) |

| | | | |
|---|---|---|---|
| C11—O3—C4—C3 | 3.2 (3) | C6—C7—C8—C9 | −19.3 (4) |
| C4—O3—C11—C12 | −179.01 (15) | C7—C8—C9—C10 | −51.0 (4) |
| O1—C1—C4—O3 | 179.95 (15) | C8—C9—C10—C1 | 81.3 (3) |
| O1—C1—C4—C3 | 0.11 (19) | O3—C11—C12—C13 | −60.0 (2) |
| C5—C1—C4—O3 | −64.9 (2) | O3—C11—C12—C17 | 118.58 (19) |
| C5—C1—C4—C3 | 115.24 (18) | C11—C12—C13—C14 | 177.65 (19) |
| C10—C1—C4—O3 | 65.0 (2) | C17—C12—C13—C14 | −1.0 (3) |
| C10—C1—C4—C3 | −114.81 (18) | C11—C12—C17—C16 | −177.78 (19) |
| O1—C1—C5—C6 | −69.6 (2) | C13—C12—C17—C16 | 0.9 (3) |
| C4—C1—C5—C6 | 179.51 (19) | C12—C13—C14—C15 | 0.6 (3) |
| C10—C1—C5—C6 | 52.3 (3) | C13—C14—C15—C16 | 0.0 (3) |
| O1—C1—C10—C9 | 60.9 (2) | C14—C15—C16—C17 | −0.1 (3) |
| C4—C1—C10—C9 | 171.67 (18) | C15—C16—C17—C12 | −0.3 (3) |
| C5—C1—C10—C9 | −61.1 (2) | | |

*Hydrogen-bond geometry (Å, º)*

Cg2 is the centroid of the benzene ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C9—H9*B*···O1 | 0.97 | 2.56 | 2.987 (3) | 106 |
| C16—H16···O2$^{i}$ | 0.93 | 2.53 | 3.362 (3) | 149 |
| C7—H7*B*···*Cg*2$^{ii}$ | 0.97 | 2.80 | 3.750 (3) | 165 |

Symmetry codes: (i) *x*+1/2, −*y*+3/2, *z*+1/2; (ii) −*x*+2, −*y*+1, −*z*+1.