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5-Phenyl-7,8-dihydro-1,3-dioxano[4,5-g]-isoquinoline

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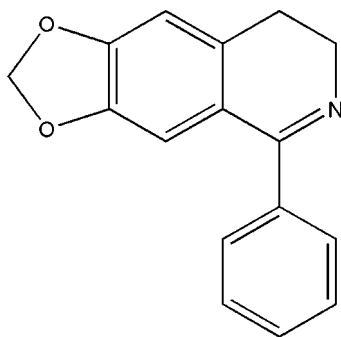
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.041; wR factor = 0.144; data-to-parameter ratio = 12.4.

In the title compound, $\text{C}_{16}\text{H}_{13}\text{NO}_2$, the two benzene rings make a dihedral angle of $55.5(2)^\circ$. The crystal packing is stabilized by intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and weak $\pi-\pi$ stacking interactions [centroid-centroid distance = $3.595(3)$ Å], linking the molecules into ladders of inversion dimers.

Related literature

For details of the biological activities of isoquinolinone compounds, see: Bentley (2000); Jayaraman *et al.* (2002). For the Bischler-Napieralski reaction, see: Bischler & Napieralski (1893). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{13}\text{NO}_2$
 $M_r = 251.27$
 Triclinic, $P\bar{1}$
 $a = 8.5005(17)$ Å
 $b = 8.5297(17)$ Å
 $c = 10.143(2)$ Å
 $\alpha = 109.07(3)^\circ$
 $\beta = 109.44(2)^\circ$
 $\gamma = 99.70(3)^\circ$
 $V = 622.9(2)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 293(2)$ K
 $0.28 \times 0.10 \times 0.08$ mm

Data collection

Rigaku R-Axis RAPID IP area-detector diffractometer
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.976$, $T_{\max} = 0.993$
 4801 measured reflections
 2145 independent reflections
 1275 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.143$
 $S = 1.13$
 2145 reflections
 173 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.20$ e Å⁻³
 $\Delta\rho_{\min} = -0.20$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{C3}-\text{H3A}\cdots\text{O2}^i$ | 0.93 | 2.55 | 3.465 (4) | 169 |

Symmetry code: (i) $-x + 1, -y, -z + 1$.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2432).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
 Bentley, K. B. (2000). *Nat. Prod. Rep.* **17**, 247–268.
 Bischler, A. & Napieralski, B. (1893). *Chem. Ber.* **26**, 1903.
 Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
 Jayaraman, M., Fox, B. M., Hollingshead, M., Kohlhagen, G., Pommier, Y. & Cushman, M. (2002). *J. Med. Chem.* **44**, 242–249.
 Rigaku (2004). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

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5-Phenyl-7,8-dihydro-1,3-dioxano[4,5-g]isoquinoline

J.-M. Li and D. Liang

Comment

Isoquinolinones are important compounds from both the synthetic and applied points of view. Their structures are incorporated in several alkaloids (Bentley, 2000) and other pharmacologically important compounds (Jayaraman *et al.*, 2002). Of the variety of methods that have been developed for the synthesis of the isoquinoline ring system, the most commonly used procedure is the Bischler-Napieralski reaction (Bischler & Napieralski, 1893). We now wish to report an effective Bischler-Napieralski procedure for the synthesis of 1,2,3,4-tetrahydro-6,7-dimethoxy-1-phenylisoquinoline the title compound (I) and report its crystal structure here.

In compound (I), all bond lengths in the molecular are normal (Allen *et al.*, 1987). The benzene ring C10–C15 and bonded atoms C7, C9, O1 and O2 are coplanar, the largest deviation from the mean plane being 0.039 (2) Å for atom O1. The other benzene ring, C1–C6, and bonded atoms C7 are also coplanar, the largest deviation from the mean plane being 0.032 (2) Å. The two benzene rings make a dihedral angle of 55.5 (2)°.

The relatively short distance of 3.595 (3) between the centroids of benzene ring C10—C15 and 1,3-dioxole ring C13/C14/C16/O1/O2 [at $-x, 1 - y, -z$] indicates the presence of weak π - π interactions, The crystal packing is stabilized by intermolecular C—H \cdots O hydrogen bonds, linking the molecules into ladders of dimers.

Experimental

The title compound was synthesized by following Bischler-Napieralski procedures: 0.01 mol N-[2-(3, 4-methylenedioxy)phenyl]benzamide (synthesized by β -(3, 4-methylenedioxy)phenethylamine, Benzoyl chloride and Et₃N) was dissolved in 20 ml CH₃CN, 5 g POCl₃ was added dropwise, the mixture was refluxed under N₂ for 5 h, after cooled the volatiles were evaporated under vacuum, then water was added and adjusted the pH to 8, after extracted with CH₂Cl₂, the organic layers was washed with saturated NaCl and dried with Na₂SO₄, the product was isolated by evaporation of the solvent and recrystallization, 2.31 g, Yield: 92%. Single crystals suitable for X-ray measurements were obtained by recrystallization from ethyl acetate at room temperature.

Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.96 Å, with $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$.

Figures

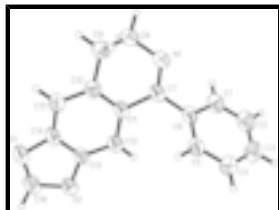


Fig. 1. The molecular structure of (I), with atom labels and 40% probability displacement ellipsoids for non-H atoms.

5-Phenyl-7,8-dihydro-1,3-dioxano[4,5-g]isoquinoline

Crystal data

$C_{16}H_{13}NO_2$

$M_r = 251.27$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.5005 (17) \text{ \AA}$

$b = 8.5297 (17) \text{ \AA}$

$c = 10.143 (2) \text{ \AA}$

$\alpha = 109.07 (3)^\circ$

$\beta = 109.44 (2)^\circ$

$\gamma = 99.70 (3)^\circ$

$V = 622.9 (2) \text{ \AA}^3$

$Z = 2$

$F_{000} = 264$

$D_x = 1.340 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1451 reflections

$\theta = 2.5\text{--}23.4^\circ$

$\mu = 0.09 \text{ mm}^{-1}$

$T = 293 (2) \text{ K}$

Block, colorless

$0.28 \times 0.10 \times 0.08 \text{ mm}$

Data collection

Rigaku R-Axis RAPID IP area-detector diffractometer

Radiation source: Rotating Anode

Monochromator: graphite

$T = 293(2) \text{ K}$

ω oscillation scans

Absorption correction: multi-scan (ABSCOR; Higashi, 1995)

$T_{\min} = 0.976$, $T_{\max} = 0.993$

4801 measured reflections

2145 independent reflections

1275 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 25.0^\circ$

$\theta_{\min} = 3.1^\circ$

$h = -10 \rightarrow 10$

$k = -10 \rightarrow 10$

$l = -11 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.144$

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.1397P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$S = 1.13$ $\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$
 2145 reflections $\Delta\rho_{\min} = -0.20 \text{ e } \text{\AA}^{-3}$
 173 parameters Extinction correction: SHELXTL (Sheldrick, 2008),
 $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
 Primary atom site location: structure-invariant direct methods Extinction coefficient: 0.048 (8)
 Secondary atom site location: difference Fourier map

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|------------|-------------|--------------|----------------------------------|
| O1 | 0.9151 (2) | 0.7157 (2) | 1.18121 (17) | 0.0688 (6) |
| O2 | 0.6920 (2) | 0.4574 (2) | 1.01260 (17) | 0.0656 (6) |
| N1 | 0.8054 (3) | 0.6182 (3) | 0.5069 (2) | 0.0638 (6) |
| C1 | 0.5553 (3) | 0.2889 (4) | 0.3031 (3) | 0.0614 (7) |
| H1B | 0.5296 | 0.3808 | 0.2795 | 0.074* |
| C2 | 0.4741 (4) | 0.1204 (4) | 0.1932 (3) | 0.0734 (8) |
| H2A | 0.3938 | 0.0996 | 0.0961 | 0.088* |
| C3 | 0.5097 (4) | -0.0172 (4) | 0.2247 (3) | 0.0772 (9) |
| H3A | 0.4550 | -0.1308 | 0.1496 | 0.093* |
| C4 | 0.6281 (4) | 0.0149 (4) | 0.3695 (3) | 0.0692 (8) |
| H4A | 0.6521 | -0.0779 | 0.3924 | 0.083* |
| C5 | 0.7107 (3) | 0.1825 (3) | 0.4798 (3) | 0.0579 (7) |
| H5A | 0.7914 | 0.2022 | 0.5765 | 0.069* |
| C6 | 0.6756 (3) | 0.3230 (3) | 0.4491 (2) | 0.0511 (6) |
| C7 | 0.7705 (3) | 0.5073 (3) | 0.5614 (2) | 0.0521 (6) |
| C8 | 0.9013 (4) | 0.7997 (3) | 0.6168 (3) | 0.0679 (8) |
| H8A | 0.8187 | 0.8570 | 0.6406 | 0.081* |
| H8B | 0.9573 | 0.8600 | 0.5702 | 0.081* |
| C9 | 1.0385 (4) | 0.8139 (3) | 0.7632 (3) | 0.0604 (7) |
| H9A | 1.1279 | 0.7664 | 0.7424 | 0.072* |
| H9B | 1.0943 | 0.9354 | 0.8351 | 0.072* |
| C10 | 0.9508 (3) | 0.7137 (3) | 0.8300 (2) | 0.0497 (6) |
| C11 | 0.8169 (3) | 0.5585 (3) | 0.7272 (2) | 0.0468 (6) |
| C12 | 0.7220 (3) | 0.4618 (3) | 0.7802 (2) | 0.0490 (6) |
| H12A | 0.6326 | 0.3575 | 0.7130 | 0.059* |

supplementary materials

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|------|------------|------------|------------|------------|
| C13 | 0.7659 (3) | 0.5266 (3) | 0.9336 (2) | 0.0492 (6) |
| C14 | 0.8994 (3) | 0.6795 (3) | 1.0347 (2) | 0.0510 (6) |
| C15 | 0.9955 (3) | 0.7752 (3) | 0.9871 (2) | 0.0525 (6) |
| H15A | 1.0871 | 0.8771 | 1.0566 | 0.063* |
| C16 | 0.7728 (4) | 0.5854 (4) | 1.1664 (3) | 0.0713 (8) |
| H16A | 0.8159 | 0.5318 | 1.2363 | 0.086* |
| H16B | 0.6882 | 0.6379 | 1.1918 | 0.086* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| O1 | 0.0833 (14) | 0.0751 (12) | 0.0399 (9) | 0.0155 (10) | 0.0240 (9) | 0.0202 (8) |
| O2 | 0.0861 (14) | 0.0677 (11) | 0.0470 (10) | 0.0158 (10) | 0.0377 (9) | 0.0221 (9) |
| N1 | 0.0805 (16) | 0.0671 (14) | 0.0497 (12) | 0.0199 (12) | 0.0329 (11) | 0.0267 (11) |
| C1 | 0.0513 (15) | 0.0779 (18) | 0.0514 (15) | 0.0196 (13) | 0.0185 (12) | 0.0255 (14) |
| C2 | 0.0562 (17) | 0.091 (2) | 0.0482 (15) | 0.0073 (15) | 0.0087 (12) | 0.0213 (15) |
| C3 | 0.080 (2) | 0.0689 (18) | 0.0552 (16) | 0.0037 (16) | 0.0187 (14) | 0.0116 (14) |
| C4 | 0.079 (2) | 0.0613 (16) | 0.0564 (16) | 0.0162 (14) | 0.0246 (14) | 0.0179 (13) |
| C5 | 0.0633 (16) | 0.0625 (15) | 0.0404 (13) | 0.0169 (13) | 0.0184 (11) | 0.0168 (12) |
| C6 | 0.0522 (15) | 0.0630 (15) | 0.0383 (12) | 0.0164 (12) | 0.0232 (10) | 0.0173 (11) |
| C7 | 0.0588 (16) | 0.0615 (15) | 0.0433 (12) | 0.0229 (12) | 0.0272 (11) | 0.0221 (12) |
| C8 | 0.087 (2) | 0.0622 (16) | 0.0626 (16) | 0.0183 (14) | 0.0396 (15) | 0.0296 (14) |
| C9 | 0.0646 (17) | 0.0594 (15) | 0.0592 (15) | 0.0142 (12) | 0.0327 (13) | 0.0223 (12) |
| C10 | 0.0498 (14) | 0.0533 (13) | 0.0471 (13) | 0.0170 (11) | 0.0226 (11) | 0.0190 (11) |
| C11 | 0.0517 (14) | 0.0525 (13) | 0.0393 (12) | 0.0180 (11) | 0.0220 (10) | 0.0186 (10) |
| C12 | 0.0533 (15) | 0.0522 (13) | 0.0427 (12) | 0.0180 (11) | 0.0221 (10) | 0.0178 (11) |
| C13 | 0.0587 (15) | 0.0553 (14) | 0.0405 (12) | 0.0199 (11) | 0.0273 (11) | 0.0202 (11) |
| C14 | 0.0596 (16) | 0.0587 (14) | 0.0359 (12) | 0.0255 (12) | 0.0197 (11) | 0.0178 (11) |
| C15 | 0.0507 (14) | 0.0560 (14) | 0.0458 (13) | 0.0150 (11) | 0.0187 (11) | 0.0171 (11) |
| C16 | 0.087 (2) | 0.0816 (19) | 0.0449 (14) | 0.0216 (16) | 0.0341 (14) | 0.0215 (14) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------|-----------|----------|-----------|
| O1—C14 | 1.370 (3) | C7—C11 | 1.481 (3) |
| O1—C16 | 1.427 (3) | C8—C9 | 1.504 (4) |
| O2—C13 | 1.381 (3) | C8—H8A | 0.9700 |
| O2—C16 | 1.421 (3) | C8—H8B | 0.9700 |
| N1—C7 | 1.283 (3) | C9—C10 | 1.499 (3) |
| N1—C8 | 1.465 (3) | C9—H9A | 0.9700 |
| C1—C2 | 1.375 (4) | C9—H9B | 0.9700 |
| C1—C6 | 1.391 (3) | C10—C11 | 1.391 (3) |
| C1—H1B | 0.9300 | C10—C15 | 1.394 (3) |
| C2—C3 | 1.368 (4) | C11—C12 | 1.406 (3) |
| C2—H2A | 0.9300 | C12—C13 | 1.359 (3) |
| C3—C4 | 1.380 (4) | C12—H12A | 0.9300 |
| C3—H3A | 0.9300 | C13—C14 | 1.376 (3) |
| C4—C5 | 1.372 (3) | C14—C15 | 1.364 (3) |
| C4—H4A | 0.9300 | C15—H15A | 0.9300 |
| C5—C6 | 1.387 (3) | C16—H16A | 0.9700 |

| | | | |
|--------------|-------------|-----------------|-------------|
| C5—H5A | 0.9300 | C16—H16B | 0.9700 |
| C6—C7 | 1.487 (3) | | |
| C14—O1—C16 | 105.44 (18) | C10—C9—C8 | 108.3 (2) |
| C13—O2—C16 | 105.24 (18) | C10—C9—H9A | 110.0 |
| C7—N1—C8 | 117.11 (19) | C8—C9—H9A | 110.0 |
| C2—C1—C6 | 120.6 (3) | C10—C9—H9B | 110.0 |
| C2—C1—H1B | 119.7 | C8—C9—H9B | 110.0 |
| C6—C1—H1B | 119.7 | H9A—C9—H9B | 108.4 |
| C3—C2—C1 | 120.9 (3) | C11—C10—C15 | 121.1 (2) |
| C3—C2—H2A | 119.6 | C11—C10—C9 | 116.9 (2) |
| C1—C2—H2A | 119.6 | C15—C10—C9 | 122.0 (2) |
| C2—C3—C4 | 119.1 (3) | C10—C11—C12 | 120.3 (2) |
| C2—C3—H3A | 120.5 | C10—C11—C7 | 117.7 (2) |
| C4—C3—H3A | 120.5 | C12—C11—C7 | 121.8 (2) |
| C5—C4—C3 | 120.5 (3) | C13—C12—C11 | 117.4 (2) |
| C5—C4—H4A | 119.7 | C13—C12—H12A | 121.3 |
| C3—C4—H4A | 119.7 | C11—C12—H12A | 121.3 |
| C4—C5—C6 | 120.9 (2) | C12—C13—C14 | 121.9 (2) |
| C4—C5—H5A | 119.6 | C12—C13—O2 | 128.3 (2) |
| C6—C5—H5A | 119.6 | C14—C13—O2 | 109.77 (19) |
| C5—C6—C1 | 118.0 (2) | C15—C14—O1 | 127.9 (2) |
| C5—C6—C7 | 122.7 (2) | C15—C14—C13 | 122.1 (2) |
| C1—C6—C7 | 119.0 (2) | O1—C14—C13 | 110.0 (2) |
| N1—C7—C11 | 122.4 (2) | C14—C15—C10 | 117.2 (2) |
| N1—C7—C6 | 116.7 (2) | C14—C15—H15A | 121.4 |
| C11—C7—C6 | 120.8 (2) | C10—C15—H15A | 121.4 |
| N1—C8—C9 | 112.5 (2) | O2—C16—O1 | 108.54 (19) |
| N1—C8—H8A | 109.1 | O2—C16—H16A | 110.0 |
| C9—C8—H8A | 109.1 | O1—C16—H16A | 110.0 |
| N1—C8—H8B | 109.1 | O2—C16—H16B | 110.0 |
| C9—C8—H8B | 109.1 | O1—C16—H16B | 110.0 |
| H8A—C8—H8B | 107.8 | H16A—C16—H16B | 108.4 |
| C6—C1—C2—C3 | -0.1 (4) | N1—C7—C11—C10 | -22.2 (4) |
| C1—C2—C3—C4 | 0.5 (5) | C6—C7—C11—C10 | 159.5 (2) |
| C2—C3—C4—C5 | -0.8 (5) | N1—C7—C11—C12 | 153.3 (3) |
| C3—C4—C5—C6 | 0.9 (4) | C6—C7—C11—C12 | -25.0 (4) |
| C4—C5—C6—C1 | -0.5 (4) | C10—C11—C12—C13 | 0.3 (4) |
| C4—C5—C6—C7 | -175.7 (2) | C7—C11—C12—C13 | -175.0 (2) |
| C2—C1—C6—C5 | 0.1 (4) | C11—C12—C13—C14 | -0.9 (4) |
| C2—C1—C6—C7 | 175.6 (2) | C11—C12—C13—O2 | 179.4 (2) |
| C8—N1—C7—C11 | 2.5 (4) | C16—O2—C13—C12 | -173.7 (3) |
| C8—N1—C7—C6 | -179.1 (2) | C16—O2—C13—C14 | 6.5 (3) |
| C5—C6—C7—N1 | 142.5 (3) | C16—O1—C14—C15 | 174.1 (3) |
| C1—C6—C7—N1 | -32.7 (3) | C16—O1—C14—C13 | -5.3 (3) |
| C5—C6—C7—C11 | -39.2 (3) | C12—C13—C14—C15 | 0.0 (4) |
| C1—C6—C7—C11 | 145.6 (2) | O2—C13—C14—C15 | 179.8 (2) |
| C7—N1—C8—C9 | 37.6 (3) | C12—C13—C14—O1 | 179.4 (2) |
| N1—C8—C9—C10 | -56.4 (3) | O2—C13—C14—O1 | -0.8 (3) |

supplementary materials

| | | | |
|-----------------|------------|-----------------|------------|
| C8—C9—C10—C11 | 37.8 (3) | O1—C14—C15—C10 | -178.0 (2) |
| C8—C9—C10—C15 | -139.8 (3) | C13—C14—C15—C10 | 1.3 (4) |
| C15—C10—C11—C12 | 1.0 (4) | C11—C10—C15—C14 | -1.8 (4) |
| C9—C10—C11—C12 | -176.6 (2) | C9—C10—C15—C14 | 175.7 (2) |
| C15—C10—C11—C7 | 176.5 (2) | C13—O2—C16—O1 | -9.7 (3) |
| C9—C10—C11—C7 | -1.1 (3) | C14—O1—C16—O2 | 9.3 (3) |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H··· <i>A</i> | <i>D</i> —H | H··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> —H··· <i>A</i> |
|--------------------------|-------------|---------------|-----------------------|-------------------------|
| C3—H3A···O2 ⁱ | 0.93 | 2.55 | 3.465 (4) | 169 |

Symmetry codes: (i) $-x+1, -y, -z+1$.

Fig. 1

