

3-(4-Hexyloxyphenyl)isobenzofuran-1(3H)-one

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Key indicators

Single-crystal X-ray study
 $T = 297$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.058
 wR factor = 0.187
Data-to-parameter ratio = 24.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

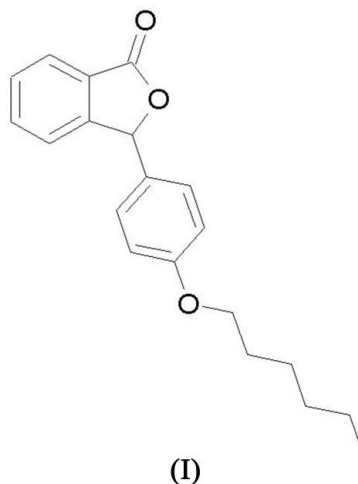
In the title compound, $\text{C}_{20}\text{H}_{22}\text{O}_3$, the hexyloxyphenyl group is orthogonal to the isobenzofuran-1-one ring system. The molecules, translated by one unit cell along the a -axis direction, are linked into a chain by intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions, and the inversion-related molecules of adjacent chains are linked *via* $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds to form a ribbon structure.

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Comment

Phthalides (isobenzofuranones) are five-membered lactones found in plants. These species possess several important properties, such as fungicidal (Aoki *et al.*, 1973; Lacova, 1974), bactericidal, herbicidal (Lacova, 1974) and analgesic activities (Elderfield, 1951). In addition, phthalide derivatives are useful in the treatment of circulatory and heart-related diseases (Bellasio, 1974). 3-Butylphthalide, a constituent of celery seed oil, exhibits anticonvulsant, antiasthmatic and antitumor properties (Veeraraghavan *et al.*, 1996). We report here the crystal structure of the title compound, (I), a phthalide derivative (Fig. 1 and Table 1).



In (I), the isobenzofuran-1-one ring system is planar, with a maximum deviation of 0.032 (1) Å for atom O1. The C9–C14 benzene ring is oriented perpendicular to the isobenzofuran-1-one ring system, with a dihedral angle of 89.13 (5)°. The hexanol group is planar within ± 0.023 (2) Å and it is almost coplanar with the C9–C14 benzene ring [the dihedral angle is 2.2 (3)°]. The bond lengths and angles in the isobenzofuran-1-one ring system are comparable to those reported for 3-(anthracen-9-yl)-3H-isobenzofuran-1-one (Palani *et al.*, 2006).

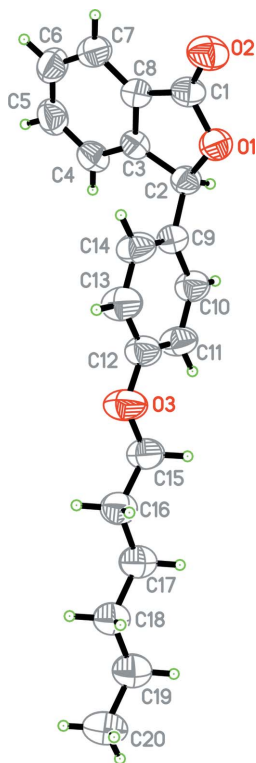


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

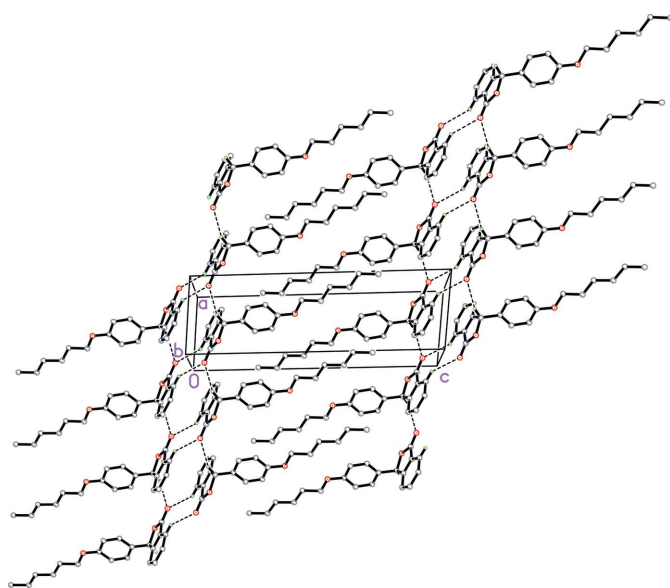


Figure 2
Part of the crystal packing of (I), showing the hydrogen-bonded (dashed lines) ribbons. H atoms not involved in hydrogen bonding have been omitted.

The bond lengths in the hexyloxyphenyl group show normal values (Allen *et al.*, 1987).

In the crystal structure, molecules translated by one unit cell along the *a*-axis direction are linked into a chain by intermolecular C2—H2···O2 hydrogen-bonding interactions

(Table 2). Inversion-related molecules of adjacent chains are linked *via* C7—H7···O2 hydrogen bonds into a ribbon structure parallel to the *a* axis (Fig. 2). In the ribbon, the isobenzofuran-1-one ring systems of the molecules at (*x*, *y*, *z*) and (1 − *x*, 1 − *y*, −*z*) are stacked in such a way that the centroid–centroid distance between their benzene rings is 3.816 (1) Å, indicating weak π–π interactions.

Experimental

Metalation of 2-bromobenzoic acid (1 g, 4.97 mmol) using a combination of dibutyl magnesium (2.6 ml, 2.6 mmol) and *n*-butyl lithium (2.2 ml, 5.46 mmol) at 253 K, followed by reaction with 4-hexyloxybenzaldehyde (1.02 g, 4.97 mmol), afforded the title compound. Single crystals suitable for X-ray diffraction were obtained from hexane by slow evaporation.

Crystal data

$C_{20}H_{22}O_3$	$V = 880.48 (10) \text{ \AA}^3$
$M_r = 310.38$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.171 \text{ Mg m}^{-3}$
$a = 6.1212 (4) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 7.7822 (5) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 19.9815 (11) \text{ \AA}$	$T = 297 (2) \text{ K}$
$\alpha = 83.225 (4)^\circ$	Block, colourless
$\beta = 83.736 (3)^\circ$	$0.27 \times 0.17 \times 0.12 \text{ mm}$
$\gamma = 69.062 (3)^\circ$	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	19069 measured reflections
ω scans	5086 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2005)	2476 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.974$, $T_{\max} = 0.991$	$R_{\text{int}} = 0.043$
	$\theta_{\max} = 30.0^\circ$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.058$	$w = 1/[\sigma^2(F_o^2) + (0.0889P)^2]$
$wR(F^2) = 0.187$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\max} = 0.001$
5086 reflections	$\Delta\rho_{\max} = 0.14 \text{ e \AA}^{-3}$
208 parameters	$\Delta\rho_{\min} = -0.18 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

O1—C1	1.365 (2)	C1—C8	1.464 (3)
O1—C2	1.461 (2)	C2—C9	1.503 (2)
O2—C1	1.200 (2)	C2—C3	1.507 (2)
O3—C12	1.365 (2)	C3—C8	1.370 (2)
O3—C15	1.420 (2)		
O3—C12—C13	115.75 (17)	O3—C12—C11	125.10 (17)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2···O2 ⁱ	0.98	2.38	3.213 (2)	143
C7—H7···O2 ⁱⁱ	0.93	2.57	3.399 (3)	148

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

The H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C–H distances of 0.93 (aromatic), 0.97 (methylene), 0.96 (methyl) and 0.98 Å (methine). The $U_{\text{iso}}(\text{H})$ values were constrained to be $1.5U_{\text{eq}}$ of the carrier atoms for methyl H atoms and $1.2U_{\text{eq}}$ for other atoms.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINTE* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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