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N-(4-Bromobenzyl)phthalimide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.007 Å
R factor = 0.047
wR factor = 0.138
Data-to-parameter ratio = 15.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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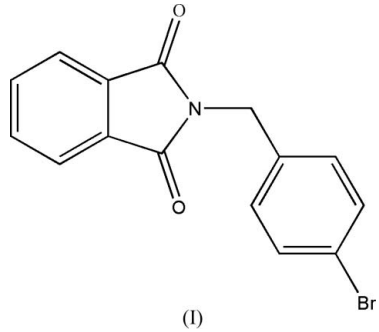
The title compound, $C_{15}H_{10}BrNO_2$, was synthesized by the reaction of 4-bromobenzyl bromide with phthalimide. The phthalimide ring system is planar and twisted with respect to the bromobenzene ring with a dihedral angle of 89.55 (17)°.

Comment

Phthalimide derivatives substituted by *N*-alkylation exhibit useful pharmaceutical properties (Chapman *et al.*, 1983; Donahoe *et al.*, 1957). The title phthalimide derivative, (I), has recently been prepared and its crystal structure is reported here.



(I)

The molecular structure of (I) is shown in Fig. 1. The phthalimide ring system is essentially planar, and twisted with respect to the C10-containing benzene ring, with a dihedral angle of 89.55 (17)°. Neighboring molecules are linked to each other *via* weak C—H···O interactions (Table 1 and Fig. 2).

Experimental

Compound (I) was prepared according to the procedure reported by Cho *et al.* (1999). Phthalimide (1 g) in a solution in dimethylformamide (20 ml) was treated with potassium carbonate (0.94 g) at room temperature for 30 min. To the stirred solution 4-bromobenzyl bromide (1.69 g) was added and the mixture was stirred at room temperature for a further 8 h. The resulting mixture was poured into water (200 ml), yielding a white precipitate. The solid product was filtered off, washed with cold water and recrystallized from ethanol, giving single crystals of (I).

Crystal data

$C_{15}H_{10}BrNO_2$
M_r = 316.15
Monoclinic, $P2_1/c$
a = 13.086 (3) Å
b = 14.174 (3) Å
c = 7.1967 (14) Å
β = 103.701 (3)°
V = 1297.0 (4) Å^3
Z = 4
D_x = 1.619 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.17 mm^{-1}
T = 294 (2) K
Block, colorless
0.24 × 0.20 × 0.14 mm

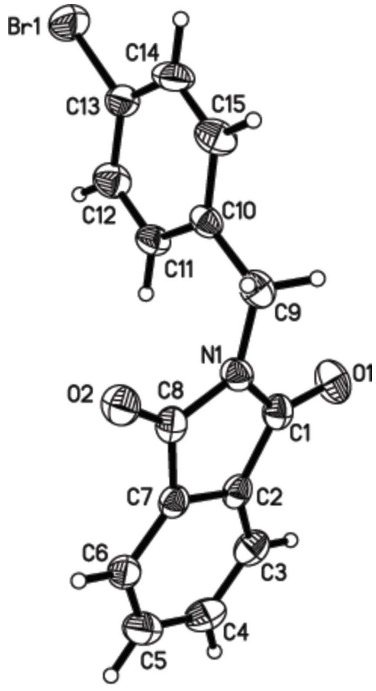


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

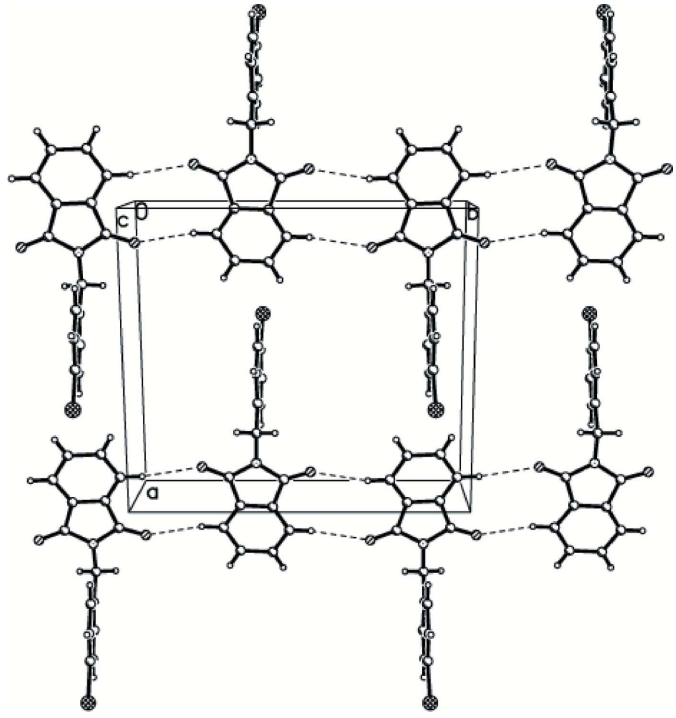


Figure 2
A packing diagram for (I), showing C—H···O interactions as dashed lines.

Data collection

Bruker SMART CCD area-detector diffractometer	7134 measured reflections
φ and ω scans	2637 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	1492 reflections with $I > 2\sigma(I)$
$T_{min} = 0.517$, $T_{max} = 0.666$	$R_{int} = 0.047$
	$\theta_{max} = 26.4^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 1.3278P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.047$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.138$	$\Delta\rho_{max} = 0.76$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -0.85$ e Å^{-3}
2637 reflections	
172 parameters	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{i}	0.93	2.57	3.491 (5)	172
C6—H6···O1^{ii}	0.93	2.44	3.360 (5)	169

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

H atoms were placed in calculated positions with C—H = 0.93 (aromatic) and 0.97 Å (methylene), and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$.

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*.

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