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N-(4-Chlorobenzyl)phthalimide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.051
wR factor = 0.158
Data-to-parameter ratio = 14.8

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

The title compound, $C_{15}H_{10}ClNO_2$, was synthesized by the reaction of 4-chlorobenzyl bromide with phthalimide. The phthalimide ring system is essentially planar and is twisted with respect to the chlorobenzene ring with a dihedral angle of 89.6 (8)°.

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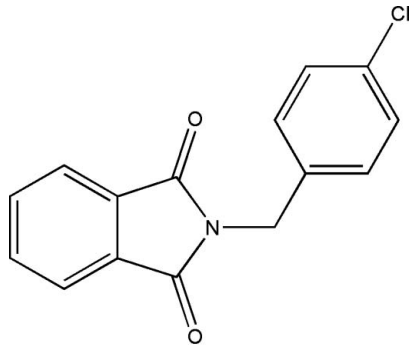
Comment

Phthalimide derivatives substituted by *N*-alkylation exhibit useful pharmaceutical properties (Chapman *et al.*, 1983; Donahoe *et al.*, 1957). The molecular structure of (I) is shown in Fig. 1. The phthalimide ring system is essentially planar, and twisted with respect to the C10–C15 benzene ring, with a dihedral angle of 89.6 (8)°. In the crystal structure, molecules are linked *via* weak intermolecular C—H···O interactions (Table 1 and Fig. 2).



(I)

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-chlorobenzyl bromide (1.39 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

$C_{15}H_{10}ClNO_2$
M_r = 271.69
Monoclinic, $P2_1/c$
a = 12.796 (5) Å
b = 14.005 (5) Å
c = 7.188 (3) Å
β = 103.763 (6)°
V = 1251.2 (8) Å^3
Z = 4
D_x = 1.442 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 294 (2) K
Block, colourless
0.22 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.937, T_{max} = 0.959
6736 measured reflections
2546 independent reflections
1102 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.158
S = 0.99
2546 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0661P)^2 + 0.1703P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{i}	0.93	2.54	3.461 (4)	169
C6—H6···O1^{ii}	0.93	2.41	3.314 (4)	165
C11—H11···O2^{iii}	0.93	2.57	3.293 (4)	135

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

H atoms were placed in calculated positions, with C—H = 0.93 (aromatic) and 0.97 Å (methylene), and refined in the riding-model approximation, 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) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

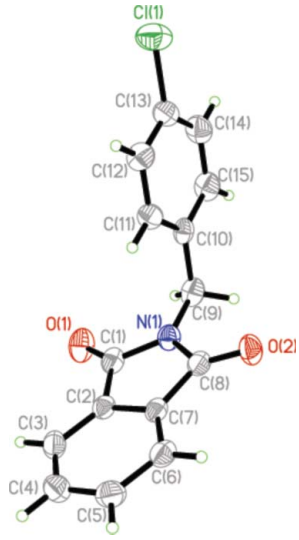


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

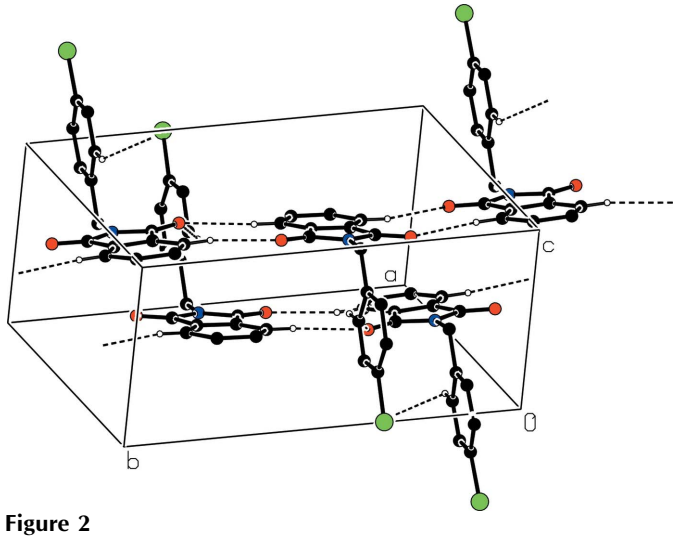


Figure 2
Part of the crystal structure of (I), showing C—H···O interactions as dashed lines.

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