The geometric parameters of the title compound, C_{11}H_{10}ClNO_{2}, are in the normal ranges. The phthalimide moiety is planar and the chloropropyl chain adopts a synclinal conformation. The crystal packing is stabilized by two intermolecular C—H···O contacts.

**Comment**

The title compound, (I), also named N-(3-chloropropyl)-phthalimide, is used as an intermediate for the synthesis of biologically active heterocycles (Kerrigan et al., 2000; Salvati et al., 2005). In view of its importance and in order to determine the conformation of this molecule, a crystal structure determination has been carried out.

A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal [Cambridge Structural Database (CSD), Version 1.7; MOGUL, Version 1.0.1; Allen, 2002]. The isoindole-1,3-dione system is planar (r.m.s. deviation = 0.011 Å). Methylene atom C9 attached to the N atom deviates from this plane by only 0.031 (1) Å. The chloropropyl moiety adopts a synclinal conformation [Cl1—C11—C10—C9 = −67.71 (12)°]. This conformation is also found for seven out of eight structures containing the Cl—CH$_2$CH$_2$CH$_2$—AA fragment (AA = any atom) retrieved from the CSD. The only
The crystal packing is stabilized by two intermolecular C—CH₂CH₂CH₂—N chain, on the other hand, adopts an anti-periplanar conformation [C11—C10—C9—N1 = 177.15 (10)°]. The crystal packing is stabilized by two intermolecular C—H⋯O contacts (Table 2).

### Experimental

A mixture of isoindole-1,3-dione (1.47 g, 10 mmol), anhydrous potassium carbonate (1.38 g, 10 mmol) and 1-bromo-3-chloropropane (1.57 g, 10 mmol) was stirred at room temperature in dimethylformamide (10 ml) for 6 h to give the title compound, which was recrystallized from methanol (m.p. 340 K).

#### Crystal data

C₁₁H₁₀ClNO₂

Mᵣ = 223.65

Monoclinic, P₂₁/n

*a* = 4.5421 (4) Å

*b* = 15.3996 (15) Å

*c* = 15.3471 (13) Å

β = 96.605 (7)°

V = 1066.35 (17) Å³

Z = 4

#### Data collection

Stoe IPDS-II two-circle
diffractometer

ω scans

Absorption correction: multi-scan
(MULABS; Spek, 2003;
Blessing, 1995)

*Tₘᵢₙ* = 0.883, *Tₘᵢₙ* = 0.930

11 334 measured reflections

**Refinement**

Refinement on *F²*

*R₁(F²) > 2σ(F²)* = 0.029

*R₁(F²) = 0.074*

*S* = 1.06

2290 reflections

157 parameters

H-atom parameters constrained

### Table 1

<table>
<thead>
<tr>
<th>Bond lengths (Å)</th>
</tr>
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<tbody>
<tr>
<td>N1—C1</td>
</tr>
<tr>
<td>N1—C4</td>
</tr>
<tr>
<td>N1—C9</td>
</tr>
<tr>
<td>Cl1—O1</td>
</tr>
<tr>
<td>Cl1—O2</td>
</tr>
<tr>
<td>Cl1—O1ii</td>
</tr>
</tbody>
</table>

### Table 2

<table>
<thead>
<tr>
<th>Hydrogen-bonding geometry (Å, °)</th>
</tr>
</thead>
<tbody>
<tr>
<td>D—H⋯A</td>
</tr>
<tr>
<td>C11—H11A—O1i</td>
</tr>
<tr>
<td>C11—H11B—O1ii</td>
</tr>
</tbody>
</table>

Symmetry codes: (i) ½ + x, ½ − y, ½ + z; (ii) −2 + x, −1 − y, 1 − z.

All H atoms were located in a difference map, but were then geometrically positioned and refined with fixed individual displacement parameters (set at 1.2 times *U*ₚₑ of the parent atom) using a riding model, with C—H = 0.95 and 0.99 Å for aromatic and methylene H atoms, respectively.

Data collection: X-AREA (Stoe & Cie, 2001); cell refinement: X-AREA; data reduction: X-AREA; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97 and PLATON.

### References


