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Structure of 3-(3,5-Dimethylpiperidino)-*N*-(*p*-Chlorophenyl)Succinimide

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Structure of 3-(3,5-Dimethylpiperidino)-*N*-(*p*-chlorophenyl)succinimide

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Abstract

In the title molecule, 3-(3,5-dimethylpiperidino)-1-(4-chlorophenyl)-2,5-pyrrolidinedione (1), the *N*-(*p*-chlorophenyl) substituent is rotated by 68.8° relative to the succinimide plane. The piperidinyl ring has a chair conformation with all substituents in equatorial positions; the conformation around the piperidino–succinimide C—N bond is staggered.

Comment

The title compound was prepared in the framework of our structural and conformational studies (Joseph-Nathan, Mendoza & Garcia G., 1972, 1974; Soriano-García, Toscano, Mendoza, García G., Guzmán, Alemán & Huipe N., 1990; Mendoza, Garcia G., Guzmán, Gutierrez & Chavez, 1991) of some 3-(1-cycloalkylamine)succinimides derived by condensation reactions from maleimides or isomaleimides and cycloalkylamines.

The chemical structure of (1) as well as its molecular stereochemistry are unequivocally established by the present X-ray investigation. The central succinimide moiety is planar within 0.004 Å. Its N atom [N(2)] has a planar-trigonal bond configuration with the *N*-(*p*-chlorophenyl) substituent, rotated by 68.8° around the C(10)—N(2) bond, out of the succinimide plane. The dimethylpiperidine substituent has a chair conformation with both methyl groups and the succinimide moiety in equatorial positions. The conformation around the N(1)—C(8) bond is staggered; all relevant torsion angles are close to 60 and 180°. The piperidine N(1) atom has a trigonal-pyramidal bond configuration; its displacement from the plane of three neighbouring atoms is 0.422 (4) Å.

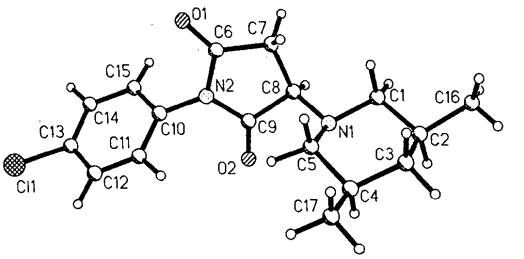

Fig. 1. General view of the title molecule (1).

Experimental

Crystal data

$C_{17}H_{21}ClN_2O_2$
M_r = 320.8
Monoclinic
$P2_1/c$
a = 8.804 (3) Å
b = 6.472 (2) Å
c = 29.075 (12) Å
β = 94.75 (2)°
V = 1651.0 (3) Å^3
Z = 4
D_x = 1.291 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 24 reflections
θ = 12–13°
μ = 0.240 mm^{-1}
T = 153 K
Needles
0.4 × 0.2 × 0.1 mm
Colourless
Crystal source: from hexane–ethyl acetate solution (2/3)

Data collection

Siemens *P3/PC* diffractometer
$\theta/2\theta$ scans
Absorption correction: none
6095 measured reflections
5773 independent reflections
1176 observed reflections [$F > 6.0\sigma(F)$]
R_{int} = 0.049
θ_{max} = 30°
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 9$
$l = -42 \rightarrow 43$
2 standard reflections monitored every 98 reflections
intensity variation: ±1.8%

Refinement

Refinement on F
Final R = 0.052
wR = 0.064
S = 2.16
1176 reflections
262 parameters
H atoms refined isotropically with fixed U_{iso} = 0.05 Å^2
$w = 1/\sigma^2(F)$
$(\Delta/\sigma)_{max}$ = 0.333
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Cl(1)	0.2122 (3)	0.2497 (4)	0.0577 (1)	0.043 (1)
O(1)	0.3922 (6)	−0.4067 (9)	0.2281 (2)	0.031 (2)
O(2)	0.0428 (6)	0.0606 (10)	0.2712 (2)	0.037 (2)
N(1)	0.1881 (7)	−0.1111 (10)	0.3580 (2)	0.024 (2)
N(2)	0.2200 (6)	−0.1508 (10)	0.2406 (2)	0.021 (2)
C(1)	0.1974 (9)	−0.2382 (15)	0.3999 (3)	0.025 (2)
C(2)	0.2038 (10)	−0.1125 (14)	0.4431 (3)	0.033 (3)
C(3)	0.3433 (10)	0.0288 (14)	0.4441 (3)	0.033 (3)
C(4)	0.3469 (9)	0.1567 (14)	0.4001 (3)	0.031 (3)
C(5)	0.3275 (9)	0.0162 (14)	0.3577 (3)	0.026 (3)
C(6)	0.3071 (8)	−0.3249 (12)	0.2535 (3)	0.024 (3)
C(7)	0.2746 (10)	−0.3854 (13)	0.3010 (3)	0.029 (3)
C(8)	0.1555 (9)	−0.2278 (15)	0.3166 (3)	0.027 (3)
C(9)	0.1281 (8)	−0.0859 (14)	0.2747 (3)	0.027 (3)
C(10)	0.2162 (9)	−0.0529 (13)	0.1967 (3)	0.024 (3)
C(11)	0.2756 (9)	0.1433 (12)	0.1920 (3)	0.025 (3)
C(12)	0.2724 (8)	0.2387 (15)	0.1511 (3)	0.027 (3)
C(13)	0.2113 (9)	0.1334 (14)	0.1123 (3)	0.031 (3)
C(14)	0.1502 (9)	−0.0647 (13)	0.1148 (3)	0.025 (3)
C(15)	0.1520 (8)	−0.1590 (14)	0.1576 (3)	0.026 (3)
C(16)	0.2134 (12)	−0.2593 (20)	0.4854 (3)	0.046 (3)
C(17)	0.4914 (9)	0.2846 (15)	0.3999 (3)	0.034 (3)

Table 2. *Geometric parameters* (Å, °)

Cl(1)—C(13)	1.758 (9)	C(3)—C(4)	1.53 (1)
O(1)—C(6)	1.22 (1)	C(4)—C(5)	1.53 (1)
O(2)—C(9)	1.21 (1)	C(4)—C(17)	1.52 (1)
N(1)—C(1)	1.47 (1)	C(6)—C(7)	1.49 (1)
N(1)—C(5)	1.48 (1)	C(7)—C(8)	1.56 (1)
N(1)—C(8)	1.43 (1)	C(8)—C(9)	1.53 (1)
N(2)—C(6)	1.40 (1)	C(10)—C(15)	1.41 (1)
N(2)—C(9)	1.40 (1)	C(11)—C(12)	1.34 (1)
N(2)—C(10)	1.42 (1)	C(12)—C(13)	1.39 (1)
C(1)—C(2)	1.50 (1)	C(13)—C(14)	1.39 (1)
C(2)—C(3)	1.53 (1)	C(14)—C(15)	1.38 (1)
C(2)—C(16)	1.55 (1)		
C(1)—N(1)—C(5)	109.1 (6)	C(6)—C(7)—C(8)	106.5 (7)
C(1)—N(1)—C(8)	113.3 (7)	N(1)—C(8)—C(7)	119.9 (6)
C(5)—N(1)—C(8)	113.5 (6)	N(1)—C(8)—C(9)	111.1 (7)
C(6)—N(2)—C(9)	112.9 (6)	C(7)—C(8)—C(9)	103.2 (6)
C(6)—N(2)—C(10)	124.9 (7)	O(2)—C(9)—N(2)	124.6 (7)
C(9)—N(2)—C(10)	122.1 (6)	O(2)—C(9)—C(8)	126.6 (7)
N(1)—C(1)—C(2)	112.9 (7)	N(2)—C(9)—C(8)	108.8 (7)
C(1)—C(2)—C(3)	108.4 (7)	N(2)—C(10)—C(11)	121.0 (7)
C(1)—C(2)—C(16)	109.3 (8)	N(2)—C(10)—C(15)	119.1 (7)
C(3)—C(2)—C(16)	111.1 (7)	C(11)—C(10)—C(15)	119.9 (7)
C(2)—C(3)—C(4)	112.3 (7)	C(10)—C(11)—C(12)	121.9 (8)
C(3)—C(4)—C(5)	110.1 (7)	C(11)—C(12)—C(13)	118.3 (9)
C(3)—C(4)—C(17)	112.0 (7)	Cl(1)—C(13)—C(12)	119.6 (7)
C(5)—C(4)—C(17)	111.0 (7)	Cl(1)—C(13)—C(14)	118.2 (6)
N(1)—C(5)—C(4)	111.4 (7)	C(12)—C(13)—C(14)	122.2 (8)
O(1)—C(6)—N(2)	122.8 (7)	C(13)—C(14)—C(15)	118.5 (8)
O(1)—C(6)—C(7)	128.7 (7)	C(10)—C(15)—C(14)	119.0 (8)
N(2)—C(6)—C(7)	108.5 (7)		

All calculations were performed with *SHELXTL-PC* (Sheldrick, 1990) programs on an IBM PC/AT computer

Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71116 (16 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: VS1003]