Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

1-(2-Chlorophenyl)-2-(isopropylamino)-ethanol

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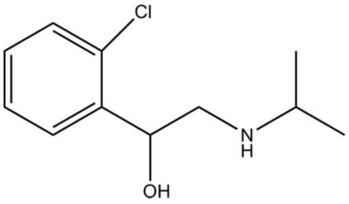
Received 30 April 2009; accepted 26 May 2009

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.043; wR factor = 0.098; data-to-parameter ratio = 20.7.

In the title compound, $C_{11}H_{16}ClNO$, the side chain of the ethylamine group is almost perpendicular to the benzene ring; the dihedral angle between the C/C/N plane of the ethylamine grouping and the benzene plane is 87.4 (2)°. An intramolecular N—H···O hydrogen bond occurs. In the crystal structure, molecules are connected weakly by O—H···N hydrogen bonds, forming a tetramer around the $\bar{4}$ symmetry axis. The tetramers are linked weakly by a C—H···O hydrogen bond.

Related literature

For a related structure, see: Koorts & Caira (1985). For the synthesis of the title compound, see; Koshinaka *et al.* (1978).



Experimental

Crystal data

$C_{11}H_{16}ClNO$
M_r = 213.70
Tetragonal, $P\bar{4}2_1c$
a = 14.0195 (5) Å
c = 12.1243 (4) Å
V = 2382.99 (14) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 296 K
0.41 × 0.38 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.871, T_{max} = 0.939
22063 measured reflections
2711 independent reflections
1796 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.098
S = 1.00
2711 reflections
131 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Absolute structure: Flack (1983), 1181 Friedel pairs
Flack parameter: 0.001 (1)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H201···N1^{i}	0.82	1.97	2.765 (3)	164
N1—H301···O1	0.86	2.25	2.789 (3)	121
C6—H6···O1^{ii}	0.93	2.45	3.283 (4)	149

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2416).

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supporting information

Acta Cryst. (2009). E**65**, o1501   [doi:10.1107/S1600536809019953]

1-(2-Chlorophenyl)-2-(isopropylamino)ethanol

Zhan Tang, Min Xu, Gui-Ru Zheng and Hai Feng

S1. Comment

The title compound (clorprenaline) is one of a series of structurally related *β*-adrenoceptorblocking drugs. Synthesis results have been reported in the literature (Koshinaka *et al.*, 1978). Clorprenaline was prepared by clorprenaline hydrochloride.

In the title compound (Fig. 1), there are no unusual bond distances or angles. The Cl atom and the phenyl plane is almost planar with the deviation of 0.0026 Å. The dihedral angle between the plane formed by C1 C2 C8 and the phenyl plane is 87.5°, which shows that the two planes are almost perpendicular. The C9—N1 distance of 1.473 (4) Å is shorter than the value of the similar bond distance of 1.502 Å (Koorts & Caira, 1985). The crystal structure indicates a possible intermolecular O—H···N interaction that might help to establish the crystal packing (Fig. 2).

S2. Experimental

Racemic clorprenaline hydrochloride (10 g, 0.047 mol), which was purchased from Hangzhou Chempro Tech Co., Inc. Hang Zhou, China, was dissolved in ethanol (100 ml) and NaOH (1.9 g, 0.047 mol) was dissolved in water (100 ml). The two solutions were mixed and the mixture was cooled for 3 h. The precipitate formed was filtered off, washed with water and dried. The crude product obtained was recrystallized from ethanol. Single crystals suitable for X-ray analysis were grown by slow evaporation at room temperature.

S3. Refinement

H atoms were placed in calculated positions and allowed to ride on their parent atoms with C—H = 0.93 (aromatic), 0.98 (methine), 0.97 (methylene), 0.96 (methyl), O—H = 0.82 and N—H = 0.858 Å, with $U_{\rm iso}$(H) = 1.2 or 1.5 times $U_{\rm eq}$ of the parent atoms.

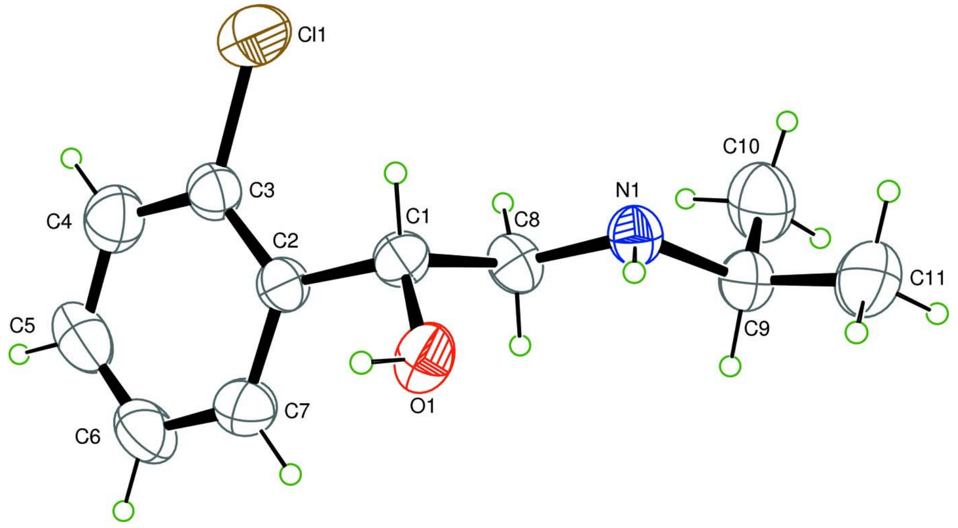

Figure 1

The molecular structure with atom labels, showing 40% probability displacement ellipsoids.

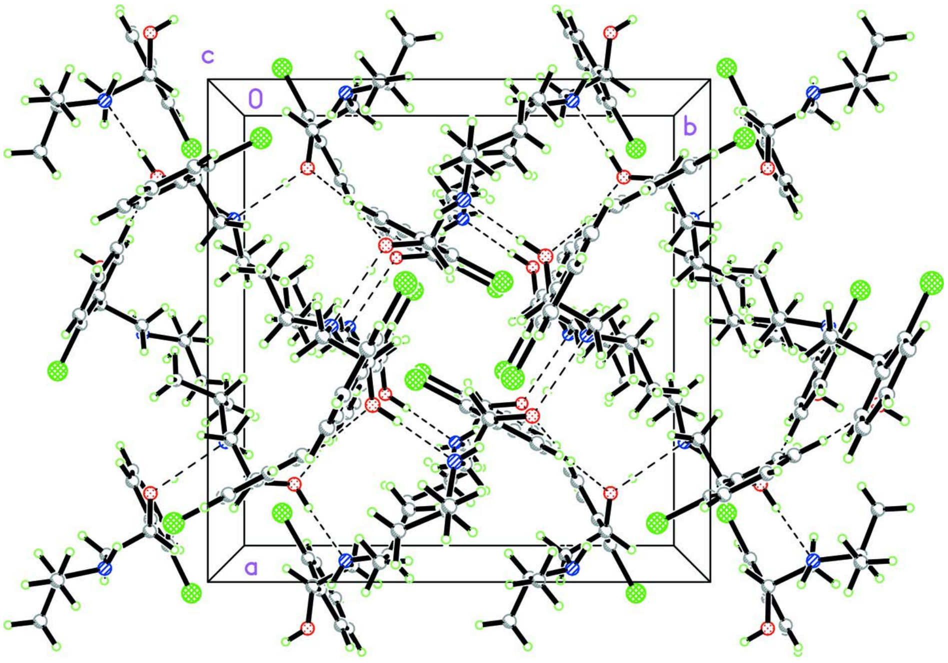

Figure 2

A packing diagram, viewed down along the *c* axis.

1-(2-Chlorophenyl)-2-(isopropylamino)ethanol

Crystal data

$C_{11}H_{16}ClNO$	V = 2382.99 (14) Å^3
M_r = 213.70	Z = 8
Tetragonal, $P\bar{4}2_1c$	F(000) = 912
Hall symbol: P -4 2n	D_x = 1.191 Mg m^{-3}
a = 14.0195 (5) Å	Mo $K\alpha$ radiation, λ = 0.71073 Å
c = 12.1243 (4) Å	Cell parameters from 13301 reflections

$\theta = 3.3–27.4°$
$\mu = 0.29\ \mathrm{mm}^{-1}$
$T = 296$ K

Block, colorless
0.41 × 0.38 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: RT
Graphite monochromator
Detector resolution: 10.00 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\mathrm{min}} = 0.871$, $T_{\mathrm{max}} = 0.939$

22063 measured reflections
2711 independent reflections
1796 reflections with $I > 2\sigma(I)$
$R_{\mathrm{int}} = 0.044$
$\theta_{\mathrm{max}} = 27.4°$, $\theta_{\mathrm{min}} = 3.3°$
$h = -18 \rightarrow 17$
$k = -18 \rightarrow 18$
$l = -13 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.098$
$S = 1.00$
2711 reflections
131 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.002P)^2 + 1.96P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\mathrm{max}} < 0.001$
$\Delta\rho_{\mathrm{max}} = 0.19$ e Å^{-3}
$\Delta\rho_{\mathrm{min}} = -0.33$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $\mathrm{Fc}^* = \mathrm{kFc}[1+0.001\mathrm{xFc}^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0308 (10)
Absolute structure: Flack (1983), 1181 Friedel pairs
Absolute structure parameter: 0.001 (1)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{\mathrm{iso}}*/U_{\mathrm{eq}}$
Cl1	0.89802 (8)	0.90968 (7)	0.76779 (8)	0.0866 (3)
O1	0.82940 (16)	1.14673 (15)	0.54268 (18)	0.0616 (6)
H201	0.8801	1.1727	0.5581	0.074*
C2	0.81036 (19)	1.07851 (19)	0.7258 (2)	0.0484 (6)
C1	0.8209 (2)	1.06095 (19)	0.6030 (2)	0.0492 (7)
H1	0.8769	1.0208	0.5896	0.059*
N1	0.74199 (17)	0.99152 (18)	0.4402 (2)	0.0527 (6)
H301	0.7679	1.0439	0.4192	0.063*
C4	0.8307 (3)	1.0339 (3)	0.9173 (3)	0.0717 (10)

H4	0.8532	0.9910	0.9697	0.086*
C3	0.8417 (2)	1.0153 (2)	0.8060 (2)	0.0557 (7)
C8	0.7325 (2)	1.0115 (2)	0.5591 (2)	0.0538 (7)
H8A	0.7227	0.9521	0.5987	0.065*
H8B	0.6772	1.0517	0.5714	0.065*
C9	0.6502 (2)	0.9762 (2)	0.3839 (3)	0.0658 (9)
H9	0.6062	1.0272	0.4054	0.079*
C7	0.7657 (2)	1.1617 (2)	0.7621 (3)	0.0649 (8)
H7	0.7436	1.2054	0.7104	0.078*
C11	0.6655 (3)	0.9809 (3)	0.2604 (3)	0.0907 (12)
H11A	0.7094	0.9319	0.2385	0.109*
H11B	0.6911	1.0422	0.2411	0.109*
H11C	0.6057	0.9717	0.2233	0.109*
C6	0.7534 (2)	1.1809 (3)	0.8735 (3)	0.0753 (10)
H6	0.7233	1.2367	0.8959	0.090*
C10	0.6073 (3)	0.8813 (3)	0.4176 (3)	0.0885 (12)
H10A	0.5965	0.8810	0.4958	0.106*
H10B	0.6505	0.8307	0.3986	0.106*
H10C	0.5479	0.8721	0.3798	0.106*
C5	0.7860 (3)	1.1172 (3)	0.9497 (3)	0.0779 (11)
H5	0.7781	1.1300	1.0244	0.093*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1254 (9)	0.0656 (5)	0.0688 (5)	0.0248 (5)	−0.0095 (6)	0.0035 (5)
O1	0.0652 (14)	0.0607 (13)	0.0588 (12)	−0.0115 (10)	−0.0115 (11)	0.0144 (10)
C2	0.0470 (14)	0.0513 (15)	0.0470 (14)	−0.0033 (12)	0.0018 (13)	−0.0009 (13)
C1	0.0505 (16)	0.0506 (16)	0.0466 (15)	0.0013 (13)	−0.0003 (13)	0.0046 (12)
N1	0.0532 (14)	0.0547 (14)	0.0501 (13)	−0.0047 (12)	−0.0052 (11)	−0.0027 (12)
C4	0.086 (3)	0.082 (3)	0.0473 (18)	−0.006 (2)	−0.0079 (17)	−0.0014 (16)
C3	0.0620 (18)	0.0542 (17)	0.0509 (16)	−0.0040 (15)	−0.0033 (14)	0.0002 (13)
C8	0.0536 (17)	0.0556 (17)	0.0522 (16)	−0.0052 (14)	0.0036 (14)	−0.0057 (14)
C9	0.0605 (19)	0.062 (2)	0.075 (2)	0.0040 (16)	−0.0155 (17)	−0.0085 (16)
C7	0.0632 (19)	0.0651 (19)	0.066 (2)	0.0135 (15)	0.0028 (17)	−0.0066 (17)
C11	0.106 (3)	0.092 (3)	0.074 (2)	0.004 (2)	−0.032 (2)	−0.007 (2)
C6	0.065 (2)	0.086 (3)	0.075 (2)	0.0079 (19)	0.0035 (19)	−0.025 (2)
C10	0.070 (2)	0.085 (3)	0.110 (3)	−0.021 (2)	−0.011 (2)	−0.007 (2)
C5	0.075 (2)	0.104 (3)	0.0548 (19)	−0.012 (2)	0.0057 (18)	−0.025 (2)

Geometric parameters (Å, º)

Cl1—C3	1.741 (3)	C8—H8B	0.9700
O1—C1	1.413 (3)	C9—C10	1.516 (5)
O1—H201	0.8200	C9—C11	1.514 (5)
C2—C3	1.387 (4)	C9—H9	0.9800
C2—C7	1.395 (4)	C7—C6	1.387 (5)
C2—C1	1.516 (4)	C7—H7	0.9300

C1—C8	1.517 (4)	C11—H11A	0.9600
C1—H1	0.9800	C11—H11B	0.9600
N1—C9	1.473 (4)	C11—H11C	0.9600
N1—C8	1.475 (4)	C6—C5	1.364 (5)
N1—H301	0.8580	C6—H6	0.9300
C4—C5	1.382 (5)	C10—H10A	0.9600
C4—C3	1.383 (4)	C10—H10B	0.9600
C4—H4	0.9300	C10—H10C	0.9600
C8—H8A	0.9700	C5—H5	0.9300

C1—O1—H201	109.5	N1—C9—C11	109.2 (3)
C3—C2—C7	117.1 (3)	C10—C9—C11	111.2 (3)
C3—C2—C1	123.6 (3)	N1—C9—H9	108.7
C7—C2—C1	119.3 (3)	C10—C9—H9	108.7
O1—C1—C8	106.1 (2)	C11—C9—H9	108.7
O1—C1—C2	112.2 (2)	C6—C7—C2	121.7 (3)
C8—C1—C2	109.8 (2)	C6—C7—H7	119.2
O1—C1—H1	109.6	C2—C7—H7	119.2
C8—C1—H1	109.6	C9—C11—H11A	109.5
C2—C1—H1	109.6	C9—C11—H11B	109.5
C9—N1—C8	113.7 (2)	H11A—C11—H11B	109.5
C9—N1—H301	110.9	C9—C11—H11C	109.5
C8—N1—H301	99.5	H11A—C11—H11C	109.5
C5—C4—C3	119.2 (3)	H11B—C11—H11C	109.5
C5—C4—H4	120.4	C5—C6—C7	119.4 (3)
C3—C4—H4	120.4	C5—C6—H6	120.3
C4—C3—C2	121.9 (3)	C7—C6—H6	120.3
C4—C3—Cl1	118.1 (3)	C9—C10—H10A	109.5
C2—C3—Cl1	120.0 (2)	C9—C10—H10B	109.5
N1—C8—C1	110.9 (2)	H10A—C10—H10B	109.5
N1—C8—H8A	109.5	C9—C10—H10C	109.5
C1—C8—H8A	109.5	H10A—C10—H10C	109.5
N1—C8—H8B	109.5	H10B—C10—H10C	109.5
C1—C8—H8B	109.5	C6—C5—C4	120.8 (3)
H8A—C8—H8B	108.1	C6—C5—H5	119.6
N1—C9—C10	110.5 (3)	C4—C5—H5	119.6

C3—C2—C1—O1	−150.5 (3)	C9—N1—C8—C1	−159.3 (3)
C7—C2—C1—O1	30.5 (4)	O1—C1—C8—N1	59.9 (3)
C3—C2—C1—C8	91.8 (3)	C2—C1—C8—N1	−178.6 (2)
C7—C2—C1—C8	−87.2 (3)	C8—N1—C9—C10	−71.4 (4)
C5—C4—C3—C2	1.0 (5)	C8—N1—C9—C11	166.0 (3)
C5—C4—C3—Cl1	−179.8 (3)	C3—C2—C7—C6	0.3 (5)
C7—C2—C3—C4	−0.9 (5)	C1—C2—C7—C6	179.4 (3)
C1—C2—C3—C4	−180.0 (3)	C2—C7—C6—C5	0.2 (5)
C7—C2—C3—Cl1	179.9 (2)	C7—C6—C5—C4	−0.2 (6)
C1—C2—C3—Cl1	0.9 (4)	C3—C4—C5—C6	−0.4 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H201···N1[i]	0.82	1.97	2.765 (3)	164
N1—H301···O1	0.86	2.25	2.789 (3)	121
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Symmetry codes: (i) *y*, −*x*+2, −*z*+1; (ii) *y*−1/2, *x*+1/2, *z*+1/2.