Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-4-Chloro-2-[(cyclopentylimino)-methyl]phenol

Lei Shi, Rui-Qin Fang, Huan-Qiu Li and Hai-Liang Zhu*

State Key Laboratory of Pharmaceutical Biotechnology, Nanjing University, Nanjing 210093, People's Republic of China
Correspondence e-mail: hailiang_zhu@163.com

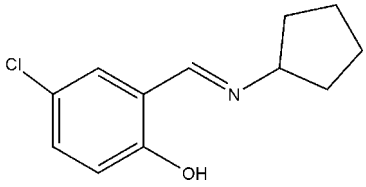
Received 27 August 2007; accepted 6 September 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.009 Å; R factor = 0.075; wR factor = 0.235; data-to-parameter ratio = 16.4.

The title molecule, $C_{12}H_{14}ClNO$, forms an intramolecular O—H···N hydrogen bond.

Related literature

For related literature, see: Allen *et al.* (1987); Li *et al.* (2006); Shi *et al.* (2007).



Experimental

Crystal data

$C_{12}H_{14}ClNO$
M_r = 223.69
Monoclinic, $C2/c$
a = 23.958 (3) Å
b = 5.5569 (12) Å
c = 21.617 (3) Å
β = 125.03 (3)°
V = 2356.5 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 293 (2) K
0.50 × 0.24 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan *SADABS* (Bruker, 2001)
T_{min} = 0.865, T_{max} = 0.965
2307 measured reflections
2251 independent reflections
908 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.075
$wR(F^2)$ = 0.235
S = 1.01
2251 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.85	2.584 (5)	148

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Measurement Foundation of Nanjing University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2134).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2001). *SMART*, *SAINT*, *SADABS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Li, Y.-G., Huang, K.-X., Ai, L. & Zhu, H.-L. (2006). *Acta Cryst.* E**62**, o2219–o2220.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Shi, L., Ge, H.-M., Tan, S.-H., Li, H.-Q., Song, Y.-C., Zhu, H.-L. & Tan, R.-X. (2007). *Eur. J. Med. Chem.* **42**, 558–564.

 doi:10.1107/S1600536807043711

supplementary materials

Acta Cryst. (2007). E**63**, o4041 [**doi:10.1107/S1600536807043711**]

(*E*)-4-Chloro-2-[(cyclopentylimino)methyl]phenol

L. Shi, R.-Q. Fang, H.-Q. Li and H.-L. Zhu

Comment

Schiff bases of salicylaldehyde and its derivatives play an important role in organic chemistry (Shi *et al.*, 2007). Recently, we have reported the structural characterization of one Schiff base compound derived from the condensation of 5-chloro-salicylaldehyde and a primary amine (Li *et al.*, 2006). As an extension of this work, we report here the crystal structure of the title compound, (I). In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). An intramolecular O—H···N hydrogen bond is formed between atoms O1 and N1.

Experimental

Cyclopentanamine (85 mg, 1 mmol) and 5-chlorosalicylaldehyde (156 mg, 1 mmol) were dissolved in methanol (10 ml) at 323 K. The mixture was stirred for 10 min to give a clear yellow solution. After keeping the solution in air for 7 d, yellow block crystals were formed at the bottom of the vessel, in about 72% yield, on slow evaporation of the solvent. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator containing anhydrous $CaCl_2$.

Refinement

All H atoms were positioned geometrically (C—H = 0.93 Å for the aromatic H atoms, C—H = 0.96 Å for the aliphatic H atoms, and O—H = 0.82 Å) and were refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.2U_{eq}(O).

Figures

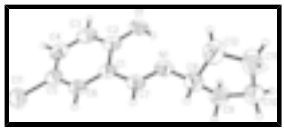


Fig. 1. The structure of the title compound (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme

(*E*)-4-Chloro-2-[(cyclopentylimino)methyl]phenol

Crystal data

$C_{12}H_{14}ClNO$	F_{000} = 944
M_r = 223.69	D_x = 1.261 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
a = 23.958 (3) Å	Cell parameters from 500 reflections
b = 5.5569 (12) Å	θ = 2.5–25.5º
c = 21.617 (3) Å	μ = 0.30 mm^{-1}
β = 125.03 (3)º	*T* = 293 (2) K

V = 2356.5 (7) Å^3	Block, yellow
Z = 8	0.50 × 0.24 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer	2251 independent reflections
Radiation source: fine-focus sealed tube	908 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 293(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan SADABS (Bruker, 2001)	h = 0→29
T_{min} = 0.865, T_{max} = 0.965	k = 0→6
2307 measured reflections	l = −26→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.075	H-atom parameters constrained
$wR(F^2)$ = 0.235	$w = 1/[\sigma^2(F_o^2) + (0.0965P)^2 + 0.6082P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
2251 reflections	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
137 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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_{iso}*/U_{eq}
C1	0.7766 (2)	0.0513 (8)	0.6790 (3)	0.0646 (12)
C2	0.8024 (3)	−0.1674 (9)	0.6717 (3)	0.0766 (13)
C3	0.8592 (3)	−0.2654 (10)	0.7361 (4)	0.0953 (17)

H3	0.8772	−0.4089	0.7325	0.114*
C4	0.8897 (3)	−0.1555 (11)	0.8053 (3)	0.0895 (16)
H4	0.9281	−0.2240	0.8478	0.107*
C5	0.8634 (3)	0.0567 (10)	0.8115 (3)	0.0798 (14)
C6	0.8080 (2)	0.1560 (9)	0.7495 (3)	0.0729 (13)
H6	0.7905	0.2986	0.7542	0.088*
C7	0.7176 (2)	0.1615 (9)	0.6126 (3)	0.0727 (13)
H7	0.7009	0.3040	0.6186	0.087*
C8	0.6300 (3)	0.1967 (10)	0.4828 (3)	0.0884 (15)
H8	0.6152	0.3291	0.5001	0.106*
C9	0.6461 (3)	0.2912 (10)	0.4289 (3)	0.0997 (17)
H9A	0.6676	0.4482	0.4448	0.120*
H9B	0.6762	0.1819	0.4261	0.120*
C10	0.5788 (3)	0.3068 (11)	0.3548 (3)	0.1093 (18)
H10A	0.5837	0.2844	0.3137	0.131*
H10B	0.5578	0.4622	0.3490	0.131*
C11	0.5366 (3)	0.1083 (15)	0.3557 (3)	0.135 (3)
H11A	0.4914	0.1676	0.3368	0.162*
H11B	0.5320	−0.0229	0.3235	0.162*
C12	0.5706 (3)	0.0228 (13)	0.4339 (3)	0.124 (2)
H12A	0.5873	−0.1402	0.4389	0.148*
H12B	0.5393	0.0251	0.4487	0.148*
Cl1	0.90235 (8)	0.1923 (3)	0.89900 (8)	0.1142 (7)
N1	0.6879 (2)	0.0740 (7)	0.5473 (3)	0.0781 (11)
O1	0.77407 (19)	−0.2775 (6)	0.6054 (2)	0.0977 (12)
H1	0.7420	−0.1970	0.5722	0.147*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.067 (3)	0.052 (3)	0.085 (3)	−0.002 (2)	0.050 (3)	0.001 (3)
C2	0.083 (3)	0.052 (3)	0.103 (4)	0.000 (3)	0.058 (3)	−0.002 (3)
C3	0.101 (4)	0.061 (4)	0.128 (5)	0.016 (3)	0.069 (4)	0.013 (4)
C4	0.082 (3)	0.080 (4)	0.098 (4)	0.007 (3)	0.046 (3)	0.024 (3)
C5	0.083 (3)	0.075 (4)	0.090 (4)	−0.006 (3)	0.054 (3)	0.006 (3)
C6	0.082 (3)	0.060 (3)	0.092 (3)	−0.005 (3)	0.059 (3)	0.000 (3)
C7	0.080 (3)	0.056 (3)	0.098 (4)	−0.001 (3)	0.060 (3)	−0.008 (3)
C8	0.081 (3)	0.089 (4)	0.088 (3)	0.015 (3)	0.045 (3)	−0.006 (3)
C9	0.096 (4)	0.088 (4)	0.108 (4)	−0.011 (3)	0.055 (4)	0.008 (3)
C10	0.111 (4)	0.101 (5)	0.107 (4)	−0.011 (4)	0.058 (4)	−0.003 (4)
C11	0.111 (5)	0.172 (7)	0.098 (4)	−0.040 (5)	0.046 (4)	−0.001 (5)
C12	0.078 (4)	0.150 (6)	0.109 (5)	−0.025 (4)	0.034 (3)	0.021 (4)
Cl1	0.1253 (13)	0.1249 (14)	0.0904 (10)	−0.0230 (10)	0.0607 (9)	−0.0078 (9)
N1	0.077 (3)	0.067 (3)	0.090 (3)	0.001 (2)	0.047 (2)	−0.005 (2)
O1	0.113 (3)	0.059 (2)	0.111 (3)	0.0075 (19)	0.057 (2)	−0.016 (2)

Geometric parameters (Å, °)

C1—C6	1.382 (6)	C8—C9	1.516 (7)

C1—C2	1.412 (6)	C8—C12	1.533 (7)
C1—C7	1.451 (6)	C8—H8	0.980
C2—O1	1.332 (5)	C9—C10	1.485 (7)
C2—C3	1.383 (7)	C9—H9A	0.970
C3—C4	1.374 (7)	C9—H9B	0.970
C3—H3	0.930	C10—C11	1.504 (8)
C4—C5	1.380 (7)	C10—H10A	0.970
C4—H4	0.930	C10—H10B	0.970
C5—C6	1.349 (6)	C11—C12	1.472 (7)
C5—Cl1	1.729 (5)	C11—H11A	0.970
C6—H6	0.930	C11—H11B	0.970
C7—N1	1.259 (5)	C12—H12A	0.970
C7—H7	0.930	C12—H12B	0.970
C8—N1	1.453 (6)	O1—H1	0.820
C6—C1—C2	119.3 (5)	C10—C9—C8	104.5 (4)
C6—C1—C7	121.2 (5)	C10—C9—H9A	110.9
C2—C1—C7	119.6 (5)	C8—C9—H9A	110.9
O1—C2—C3	120.1 (5)	C10—C9—H9B	110.9
O1—C2—C1	122.0 (5)	C8—C9—H9B	110.9
C3—C2—C1	117.9 (5)	H9A—C9—H9B	108.9
C4—C3—C2	121.4 (5)	C9—C10—C11	105.4 (5)
C4—C3—H3	119.3	C9—C10—H10A	110.7
C2—C3—H3	119.3	C11—C10—H10A	110.7
C3—C4—C5	119.9 (5)	C9—C10—H10B	110.7
C3—C4—H4	120.0	C11—C10—H10B	110.7
C5—C4—H4	120.0	H10A—C10—H10B	108.8
C6—C5—C4	119.7 (5)	C12—C11—C10	108.5 (5)
C6—C5—Cl1	121.0 (5)	C12—C11—H11A	110.0
C4—C5—Cl1	119.3 (5)	C10—C11—H11A	110.0
C5—C6—C1	121.7 (5)	C12—C11—H11B	110.0
C5—C6—H6	119.1	C10—C11—H11B	110.0
C1—C6—H6	119.1	H11A—C11—H11B	108.4
N1—C7—C1	123.3 (5)	C11—C12—C8	105.7 (5)
N1—C7—H7	118.3	C11—C12—H12A	110.6
C1—C7—H7	118.3	C8—C12—H12A	110.6
N1—C8—C9	112.1 (4)	C11—C12—H12B	110.6
N1—C8—C12	111.3 (5)	C8—C12—H12B	110.6
C9—C8—C12	103.5 (4)	H12A—C12—H12B	108.7
N1—C8—H8	109.9	C7—N1—C8	120.6 (4)
C9—C8—H8	109.9	C2—O1—H1	109.5
C12—C8—H8	109.9		
C6—C1—C2—O1	179.6 (4)	C6—C1—C7—N1	179.2 (4)
C7—C1—C2—O1	0.0 (6)	C2—C1—C7—N1	−1.2 (7)
C6—C1—C2—C3	−1.1 (6)	N1—C8—C9—C10	155.3 (4)
C7—C1—C2—C3	179.2 (4)	C12—C8—C9—C10	35.3 (6)
O1—C2—C3—C4	179.7 (5)	C8—C9—C10—C11	−31.1 (6)
C1—C2—C3—C4	0.4 (7)	C9—C10—C11—C12	14.8 (8)
C2—C3—C4—C5	0.4 (8)	C10—C11—C12—C8	7.3 (8)

C3—C4—C5—C6	−0.4 (7)	N1—C8—C12—C11	−146.6 (5)
C3—C4—C5—Cl1	179.9 (4)	C9—C8—C12—C11	−26.1 (7)
C4—C5—C6—C1	−0.3 (7)	C1—C7—N1—C8	−178.5 (4)
Cl1—C5—C6—C1	179.4 (3)	C9—C8—N1—C7	112.8 (5)
C2—C1—C6—C5	1.1 (7)	C12—C8—N1—C7	−131.9 (5)
C7—C1—C6—C5	−179.2 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.85	2.584 (5)	148

Fig. 1