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N′-[1-(4-Chlorophenyl)ethylidene]-propionohydrazide

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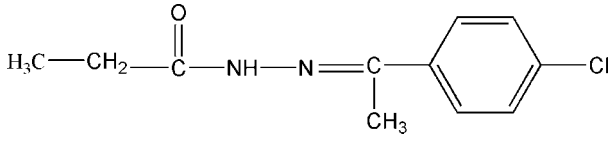
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.121; data-to-parameter ratio = 16.6.

The title compound, $C_{11}H_{13}ClN_2O$, was prepared by reacting *p*-chloroacetophenone and propionylhydrazine. Molecules are associated in centrosymmetric dimers through N—H···O hydrogen bonds involving amine and carbonyl groups.

Related literature

For analytical applications of Schiff bases, see: Cimerman *et al.* (1997). For related structures, see: Sutherland & Hoy (1968); Tucker *et al.* (1975).



Experimental

Crystal data

$C_{11}H_{13}ClN_2O$
M_r = 224.68
Monoclinic, $P2_1/c$
a = 7.8599 (14) Å
b = 8.1421 (15) Å
c = 17.901 (4) Å
β = 98.172 (3)°
V = 1134.0 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 294 (2) K
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.929, T_{max} = 0.946
6276 measured reflections
2310 independent reflections
1537 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.121
S = 1.01
2310 reflections
139 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1^{i}	0.86	2.13	2.9744 (19)	166

Symmetry code: (i) $-x+1, -y+2, -z$.

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); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2131).

References

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supplementary materials

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N'-[1-(4-Chlorophenyl)ethylidene]propionohydrazide

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Comment

Schiff bases have received considerable attention in the literature. They are attractive from several points of view, such as the possibility of analytical applications (Cimerman *et al.*, 1997). As part of our search for new Schiff bases, we synthesized the title compound (Fig. 1) and describe its structure here. Bond lengths and angles in the benzene ring are as expected. The bond length C7═N1, 1.279 (2) Å is similar to that reported in related imines (*e.g.* 1.287 Å, Tucker *et al.*, 1975). The bond length for the carbonyl group C9═O1, 1.222 (2) Å is shorter than that observed in 4-acetyl-2'-chlorobiphenyl (1.298 Å, Sutherland & Hoy, 1968).

Regarding the crystal structure, the molecules are connected into centrosymmetric dimers through hydrogen bonds involving amine group N2—H2 and carbonyl group C9═O1.

Experimental

p-Chloroacetophenone (0.1 mol) and propionylhydrazine (0.1 mol) were mixed in ethanol (30 ml) and refluxed for 5 h. Then the mixture was poured into water to afford colorless solids. The solids were filtrated and washed with water. Finally, the resulting crystals were dried at 298 K. Single crystals suitable for X-ray measurements were obtained by recrystallization from EtOH at room temperature.

Refinement

H atoms were placed in idealized positions and allowed to ride on their carrier atom, with N—H and C—H distances fixed to 0.86 (amine NH), 0.93 (aromatic CH), 0.97 (methylene CH_2) or 0.98 Å (methyl CH_3). Isotropic displacement parameters for H atoms were fixed to $U_{iso}(H) = xU_{eq}$(carrier atom) with $x = 1.5$ for methyl groups and $x = 1.2$ otherwise.

Figures

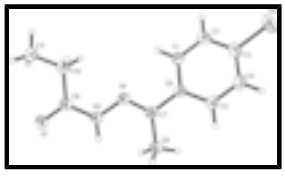

Fig. 1. The structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

N'-[1-(4-Chlorophenyl)ethylidene]propionohydrazide

Crystal data

$C_{11}H_{13}ClN_2O$	$Z = 4$
$M_r = 224.68$	$F_{000} = 472$

Monoclinic, $P2_1/c$	D_x = 1.316 Mg m^{-3}
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.8599 (14) Å	θ = 2.3–26.4º
b = 8.1421 (15) Å	μ = 0.31 mm^{-1}
c = 17.901 (4) Å	T = 294 (2) K
β = 98.172 (3)º	Block, colourless
V = 1134.0 (4) Å^3	0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2310 independent reflections
Radiation source: fine-focus sealed tube	1537 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −5→9
T_{min} = 0.929, T_{max} = 0.946	k = −9→10
6276 measured reflections	l = −22→20

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.039	$w = 1/[\sigma^2(F_o^2) + (0.0624P)^2 + 0.1491P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.121	$(\Delta/\sigma)_{max} < 0.001$
S = 1.01	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
2310 reflections	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
139 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.055 (5)
Secondary atom site location: difference Fourier map	

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	−0.49633 (7)	1.01474 (8)	0.27988 (4)	0.0772 (3)
O1	0.46696 (17)	0.79643 (17)	−0.02491 (9)	0.0649 (4)
N1	0.15576 (17)	0.92409 (17)	0.08275 (8)	0.0420 (4)
N2	0.29715 (18)	0.92652 (18)	0.04509 (9)	0.0465 (4)
H2	0.3601	1.0132	0.0467	0.056*
C1	−0.1647 (2)	0.9348 (2)	0.13482 (10)	0.0445 (4)
H1	−0.1574	0.8660	0.0939	0.053*

C2	−0.3068 (2)	0.9252 (2)	0.17216 (11)	0.0503 (5)
H2A	−0.3944	0.8509	0.1564	0.060*
C3	−0.3174 (2)	1.0267 (2)	0.23282 (11)	0.0505 (5)
C4	−0.1886 (3)	1.1367 (3)	0.25700 (12)	0.0618 (6)
H4	−0.1959	1.2042	0.2983	0.074*
C5	−0.0481 (3)	1.1452 (3)	0.21879 (11)	0.0558 (5)
H5	0.0387	1.2201	0.2348	0.067*
C6	−0.0326 (2)	1.0455 (2)	0.15733 (10)	0.0404 (4)
C7	0.1197 (2)	1.0550 (2)	0.11680 (10)	0.0409 (4)
C8	0.2186 (3)	1.2134 (2)	0.11785 (12)	0.0600 (6)
H8A	0.3273	1.2011	0.1494	0.090*
H8B	0.1542	1.2996	0.1374	0.090*
H8C	0.2374	1.2404	0.0675	0.090*
C9	0.3376 (2)	0.7939 (2)	0.00572 (10)	0.0458 (5)
C10	0.2204 (3)	0.6472 (2)	0.00174 (12)	0.0586 (5)
H10A	0.1022	0.6848	−0.0050	0.070*
H10B	0.2414	0.5883	0.0493	0.070*
C11	0.2442 (3)	0.5312 (3)	−0.06134 (14)	0.0675 (6)
H11A	0.2359	0.5910	−0.1079	0.101*
H11B	0.1566	0.4482	−0.0653	0.101*
H11C	0.3552	0.4803	−0.0510	0.101*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0663 (4)	0.0794 (4)	0.0954 (5)	0.0172 (3)	0.0438 (3)	0.0202 (3)
O1	0.0600 (9)	0.0453 (8)	0.0979 (11)	−0.0064 (6)	0.0402 (8)	−0.0063 (7)
N1	0.0439 (8)	0.0404 (8)	0.0435 (8)	−0.0031 (6)	0.0120 (6)	0.0015 (7)
N2	0.0467 (9)	0.0376 (8)	0.0586 (10)	−0.0073 (7)	0.0189 (7)	−0.0005 (7)
C1	0.0506 (11)	0.0410 (9)	0.0424 (10)	−0.0036 (8)	0.0079 (8)	−0.0012 (8)
C2	0.0461 (10)	0.0467 (10)	0.0579 (12)	−0.0048 (8)	0.0063 (9)	0.0064 (9)
C3	0.0500 (11)	0.0493 (11)	0.0557 (12)	0.0093 (9)	0.0195 (9)	0.0121 (9)
C4	0.0781 (15)	0.0562 (12)	0.0559 (13)	−0.0004 (11)	0.0262 (11)	−0.0107 (10)
C5	0.0619 (12)	0.0531 (11)	0.0546 (12)	−0.0126 (10)	0.0158 (9)	−0.0144 (10)
C6	0.0457 (10)	0.0358 (9)	0.0402 (10)	−0.0014 (7)	0.0078 (7)	0.0015 (7)
C7	0.0472 (10)	0.0350 (9)	0.0406 (10)	−0.0038 (8)	0.0065 (7)	0.0017 (8)
C8	0.0616 (13)	0.0425 (11)	0.0810 (15)	−0.0108 (9)	0.0272 (11)	−0.0053 (10)
C9	0.0463 (10)	0.0384 (10)	0.0555 (11)	−0.0024 (8)	0.0170 (9)	0.0024 (8)
C10	0.0627 (12)	0.0481 (11)	0.0700 (13)	−0.0136 (10)	0.0268 (10)	−0.0078 (10)
C11	0.0701 (15)	0.0538 (12)	0.0822 (17)	−0.0087 (10)	0.0234 (12)	−0.0154 (11)

Geometric parameters (Å, °)

Cl1—C3	1.7417 (19)	C5—C6	1.387 (3)
O1—C9	1.222 (2)	C5—H5	0.9300
N1—C7	1.279 (2)	C6—C7	1.487 (2)
N1—N2	1.3794 (19)	C7—C8	1.505 (2)
N2—C9	1.352 (2)	C8—H8A	0.9600
N2—H2	0.8600	C8—H8B	0.9600

C1—C2	1.383 (2)	C8—H8C	0.9600
C1—C6	1.391 (2)	C9—C10	1.504 (2)
C1—H1	0.9300	C10—C11	1.504 (3)
C2—C3	1.376 (3)	C10—H10A	0.9700
C2—H2A	0.9300	C10—H10B	0.9700
C3—C4	1.375 (3)	C11—H11A	0.9600
C4—C5	1.381 (3)	C11—H11B	0.9600
C4—H4	0.9300	C11—H11C	0.9600
C7—N1—N2	118.00 (14)	N1—C7—C8	124.80 (16)
C9—N2—N1	120.59 (14)	C6—C7—C8	119.26 (15)
C9—N2—H2	119.7	C7—C8—H8A	109.5
N1—N2—H2	119.7	C7—C8—H8B	109.5
C2—C1—C6	121.17 (17)	H8A—C8—H8B	109.5
C2—C1—H1	119.4	C7—C8—H8C	109.5
C6—C1—H1	119.4	H8A—C8—H8C	109.5
C3—C2—C1	119.43 (17)	H8B—C8—H8C	109.5
C3—C2—H2A	120.3	O1—C9—N2	119.52 (16)
C1—C2—H2A	120.3	O1—C9—C10	122.38 (16)
C4—C3—C2	120.99 (18)	N2—C9—C10	118.10 (15)
C4—C3—Cl1	119.55 (16)	C9—C10—C11	113.18 (17)
C2—C3—Cl1	119.45 (16)	C9—C10—H10A	108.9
C3—C4—C5	118.78 (19)	C11—C10—H10A	108.9
C3—C4—H4	120.6	C9—C10—H10B	108.9
C5—C4—H4	120.6	C11—C10—H10B	108.9
C4—C5—C6	122.06 (18)	H10A—C10—H10B	107.8
C4—C5—H5	119.0	C10—C11—H11A	109.5
C6—C5—H5	119.0	C10—C11—H11B	109.5
C5—C6—C1	117.56 (17)	H11A—C11—H11B	109.5
C5—C6—C7	121.64 (16)	C10—C11—H11C	109.5
C1—C6—C7	120.80 (16)	H11A—C11—H11C	109.5
N1—C7—C6	115.93 (15)	H11B—C11—H11C	109.5
C7—N1—N2—C9	−177.47 (17)	N2—N1—C7—C6	−179.27 (14)
C6—C1—C2—C3	−0.2 (3)	N2—N1—C7—C8	1.1 (3)
C1—C2—C3—C4	−0.3 (3)	C5—C6—C7—N1	153.78 (18)
C1—C2—C3—Cl1	180.00 (14)	C1—C6—C7—N1	−25.9 (2)
C2—C3—C4—C5	0.7 (3)	C5—C6—C7—C8	−26.5 (3)
Cl1—C3—C4—C5	−179.65 (16)	C1—C6—C7—C8	153.74 (17)
C3—C4—C5—C6	−0.5 (3)	N1—N2—C9—O1	−177.32 (16)
C4—C5—C6—C1	0.0 (3)	N1—N2—C9—C10	2.4 (3)
C4—C5—C6—C7	−179.69 (18)	O1—C9—C10—C11	−18.3 (3)
C2—C1—C6—C5	0.3 (3)	N2—C9—C10—C11	161.97 (18)
C2—C1—C6—C7	−179.95 (16)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.86	2.13	2.9744 (19)	166

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*.

Fig. 1