

1-(4-Chlorophenyl)propane-1,2-dione
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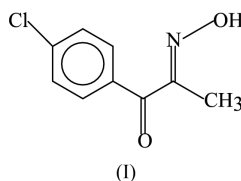
Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.042
 wR factor = 0.125
Data-to-parameter ratio = 15.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title molecule, $\text{C}_9\text{H}_8\text{NO}_2\text{Cl}$, the dihedral angle between the aromatic ring and propan-2-one oxime moiety is $54.05(4)^\circ$. In the crystal structure, the molecules exist as $\text{O}-\text{H}\cdots\text{N}$ hydrogen-bonded dimers around the inversion centres.

Comment

The title compound, (I), is an α -oximino ketone. Recently, we have developed a simple method for the preparation of α -oximino ketones (Mohammed & Nagendrappa, 2003), which finds many applications in organic synthesis. It also serves as ligand for transition metal complexes. The oxime group in this compound is potentially ambidentate with possibilities of coordination through the N and/or O atom. Here we report its structure.



The title molecule (Fig. 1) is non-planar, with two planar segments in it, *viz.* the chlorophenyl ring and the $\text{C}1-\text{C}2-\text{C}3-\text{N}2-\text{O}2$ plane; the dihedral angle between them is $54.05(4)^\circ$. The $\text{C}=\text{O}$ group is almost *cis* with respect to the $\text{C}7-\text{C}8$ bond, the torsion angle $\text{C}8-\text{C}7-\text{C}1-\text{O}1$ being $35.9(2)^\circ$; it is also nearly *trans* to the oxime group [$\text{N}2-\text{C}2-\text{C}1-\text{O}1 = -159.49(15)^\circ$]. The geometrical parameters of the oxime group are comparable with the corresponding values found in other reported oximes (Saarinen & Korvenranta, 1975; Bertolasi *et al.*, 1982; Ciajolo *et al.*, 1981; Hutton *et al.*, 1979). An intramolecular $\text{C}-\text{H}\cdots\text{O}$ interaction involving the carbonyl O atom is observed.

In the crystal structure, the inversion-related molecules are $\text{O}-\text{H}\cdots\text{N}$ hydrogen-bonded through their oxime groups to form dimers (Fig. 2 and Table 2). These hydrogen bonds form rings of graph-set motif $R_2^2(6)$. Within the dimer, the hydroxyl O atoms are involved in weak $\text{O}-\text{H}\cdots\text{O}$ interactions to form rings of graph-set motif $R_2^2(4)$. It is noteworthy that a significantly short $\text{Cl}\cdots\text{Cl}$ contact of $3.408(1)\text{ \AA}$ is observed between $\text{Cl}1(-x, -y, 1-z)$.

Experimental

The title compound was synthesized by the method reported by Mohammed & Nagendrappa (2003). Crystals were grown by slow evaporation of a chloroform solution.

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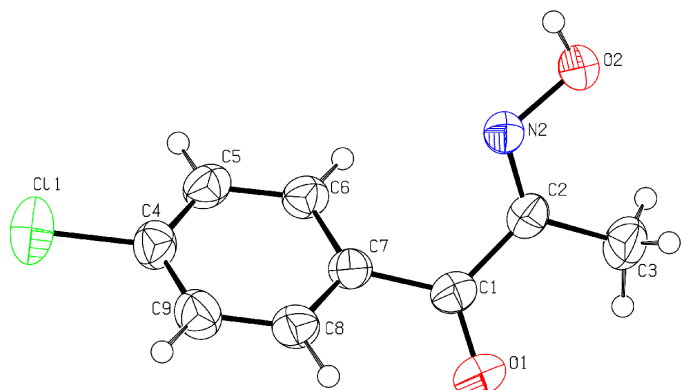


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

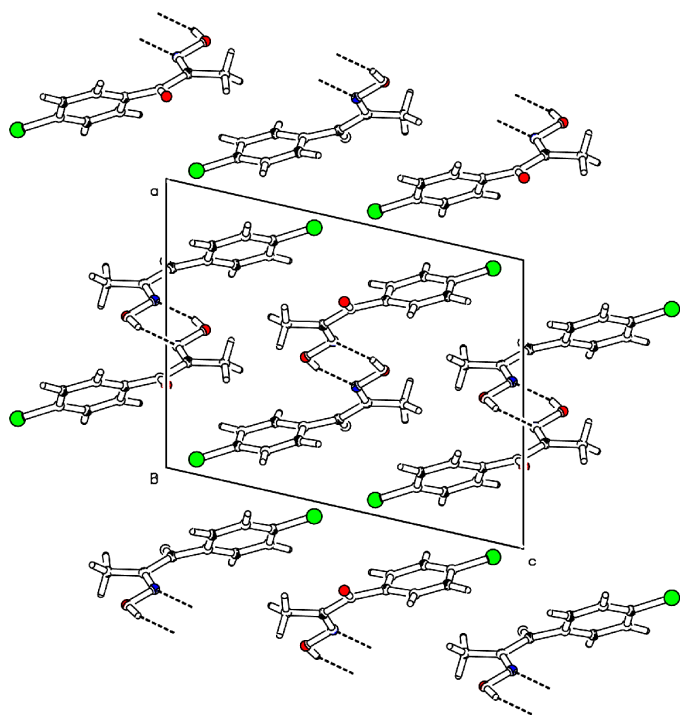


Figure 2
The molecular packing in the title compound, viewed down the *b* axis, showing O—H...N hydrogen-bonded dimers.

Crystal data

$C_9H_8ClNO_2$
 $M_r = 197.61$
Monoclinic, $P2_1/c$
 $a = 11.066$ (2) Å
 $b = 5.9348$ (13) Å
 $c = 14.075$ (3) Å
 $\beta = 102.809$ (4)°
 $V = 901.4$ (3) Å³
 $Z = 4$

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.930$, $T_{\max} = 0.964$
7478 measured reflections

$D_x = 1.456$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 7478 reflections
 $\theta = 1.9$ – 28.0°
 $\mu = 0.39$ mm⁻¹
 $T = 293$ (2) K
Plate, colorless
 $0.3 \times 0.2 \times 0.1$ mm

2116 independent reflections
1827 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$
 $\theta_{\text{max}} = 28.0^\circ$
 $h = -14 \rightarrow 13$
 $k = -7 \rightarrow 7$
 $l = -18 \rightarrow 18$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.125$
 $S = 0.95$
2116 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0784P)^2 + 0.2853P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.21$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³
Extinction correction: SHELXL97
Extinction coefficient: 0.043 (5)

Table 1

Selected geometric parameters (Å, °).

Cl1—C4	1.7330 (16)	C1—C7	1.491 (2)
O1—C1	1.2138 (19)	C1—C2	1.499 (2)
O2—N2	1.3906 (16)	C2—C3	1.491 (2)
N2—C2	1.2801 (19)		
C2—N2—O2	112.17 (12)	N2—C2—C1	116.11 (13)
N2—C2—C3	125.21 (14)	C3—C2—C1	118.49 (14)

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2—H2...N2 ⁱ	0.82 (2)	2.04 (2)	2.830 (2)	163 (2)
O2—H2...O2 ⁱ	0.82 (2)	2.62 (2)	3.219 (2)	131 (2)
C3—H3B...O1	0.96	2.43	2.815 (2)	103

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

The methyl H atoms were positioned geometrically [$C-H = 0.96$ Å and $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(C)$] and a rotating group model was used for their refinement. The remaining H atoms were located in a difference Fourier map and their parameters (x , y , z and U_{iso}) were refined. The C—H distances are in the range 0.90 (2)–0.97 (3) Å and the O—H distance is 0.82 (2) Å.

Data collection: SMART (Bruker, 1998); cell refinement: SMART; data reduction: SAINT (Bruker, 1998); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: PLATON.

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