

1-Chloro-1-[(4-chlorophenyl)hydrazinylidene]propan-2-one

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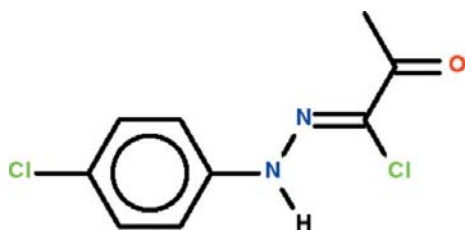
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.070; wR factor = 0.208; data-to-parameter ratio = 14.6.

The non-H atoms of the title compound, $\text{C}_9\text{H}_8\text{Cl}_2\text{N}_2\text{O}$, lie nearly on a plane (r.m.s. deviation = 0.110 Å), and the $\text{C}=\text{N}$ double bond has a Z configuration. In the crystal, adjacent molecules are linked by an $\text{N}-\text{H}\cdots\text{O}_{\text{carbonyl}}$ hydrogen bond, forming a chain running along [100].

Related literature

For the synthesis, see: Benincori *et al.* (1990); Sayed *et al.* (2002). For background to the title compound, see: Asiri *et al.* (2010).



Experimental

Crystal data

$\text{C}_9\text{H}_8\text{Cl}_2\text{N}_2\text{O}$

$M_r = 231.07$

Monoclinic, $P2_1/c$
 $a = 5.7558$ (4) Å
 $b = 23.3282$ (17) Å
 $c = 7.4107$ (6) Å
 $\beta = 96.976$ (7)°
 $V = 987.69$ (13) Å³

$Z = 4$
Cu $K\alpha$ radiation
 $\mu = 5.65$ mm⁻¹
 $T = 100$ K
 $0.35 \times 0.05 \times 0.03$ mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
 $T_{\text{min}} = 0.243$, $T_{\text{max}} = 0.849$

3486 measured reflections
1939 independent reflections
1640 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.070$
 $wR(F^2) = 0.208$
 $S = 1.17$
1939 reflections
133 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 1.28$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.54$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2}\cdots\text{O1}^i$	0.85 (8)	2.26 (8)	3.029 (6)	150 (7)

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5260).

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