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Ethyl 2-chloro-[2-(4-chlorophenyl)-hydrazin-1-ylidene]acetate

Abdullah M. Asiri,[a] Mohie E. M. Zayed[a] and Seik Weng Ng[b]*

[a]Chemistry Department, Faculty of Science, King Abdul Aziz University, PO Box 80203, Jeddah 21589, Saudi Arabia, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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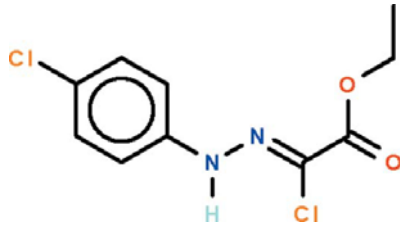
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.007 Å; R factor = 0.072; wR factor = 0.188; data-to-parameter ratio = 17.4.

The title compound, $C_{10}H_{10}Cl_2N_2O_2$, features a planar C_{ar}—N(H)—N=C(Cl) unit [torsion angle = 5.5 (4)°] whose benzene substituent is coplanar with it [dihedral angle = 4.7 (4)°]; this unit is slightly twisted with respect to the carboxyl –CO_2 fragment [dihedral angle = 2.2 (52)°]. The amino group acts as a hydrogen-bond donor to the carbonyl O atom of an adjacent molecule; the hydrogen bond generates a helical polymer that runs along the b axis of the monoclinic unit cell.

Related literature

For a review of the reactions of hydrazonyl halides with heterocyclic thiones for heteroannulation, the synthesis of spiroheterocycles and heterocyclic ring formation, see: Shawali & Farghaly (2008). For related structures, see: Xu (2006); Yin *et al.* (2006).



Experimental

Crystal data

$C_{10}H_{10}Cl_2N_2O_2$
M_r = 261.10
Monoclinic, $P2_1$
a = 4.4611 (7) Å
b = 9.4546 (14) Å
c = 13.464 (2) Å
β = 91.642 (2)°
V = 567.65 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.56 mm^{-1}
T = 100 K
0.35 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.829, T_{max} = 0.973
5298 measured reflections
2518 independent reflections
2191 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.188
S = 1.03
2518 reflections
145 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack (1983), 1123 Friedel pairs
Flack parameter: 0.03 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.20	3.009 (5)	156

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; 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: NK2055).

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