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Ethyl (*Z*)-2-chloro-2-(2-phenylhydrazin-1-ylidene)acetate

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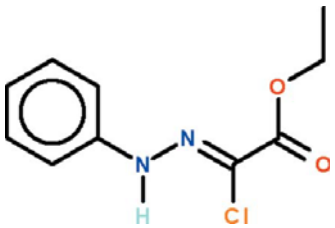
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.026; wR factor = 0.076; data-to-parameter ratio = 17.1.

The title compound, $C_{10}H_{11}ClN_2O_2$, features an almost planar C_{ar}—N(H)—N=C(Cl) unit [torsion angle = 0.8 (1)° whose phenyl substituent is almost coplanar with it [dihedral angle = 2.8 (2)°]; this unit is slightly twisted with respect to the carboxyl –CO_2 fragment [dihedral angle = 10.3 (2)°]. In the crystal, the amino group acts as a hydrogen-bond donor to the carbonyl O atom of an adjacent molecule; the hydrogen bond generates a helical chain 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 crystal structures, see: Xu (2006); Yin *et al.* (2006).



Experimental

Crystal data

$C_{10}H_{11}ClN_2O_2$
M_r = 226.66
Monoclinic, $P2_1/c$
a = 10.5091 (7) Å
b = 11.1813 (8) Å
c = 10.1190 (7) Å
β = 118.148 (1)°
V = 1048.41 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 100 K
0.30 × 0.30 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.904, T_{max} = 0.966
6532 measured reflections
2399 independent reflections
2191 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.076
S = 1.03
2399 reflections
140 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.85 (1)	2.18 (1)	2.969 (1)	153 (2)

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

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: NK2054).

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