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

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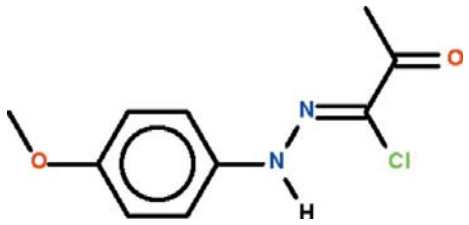
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.102; data-to-parameter ratio = 14.7.

The non-H atoms of the title compound, $C_{10}H_{11}ClN_2O_2$, lie nearly on a plane (r.m.s. deviation = 0.150 Å), and the C=N double bond has a Z configuration. In the crystal, adjacent molecules are linked by an N—H···$O_{carbonyl}$ hydrogen bond, forming a chain running along [201].

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

$C_{10}H_{11}ClN_2O_2$
M_r = 226.66
Monoclinic, $P2_1/c$
a = 5.8873 (3) Å
b = 25.0467 (10) Å
c = 7.3041 (3) Å
β = 99.016 (4)°
V = 1063.74 (8) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 3.05 mm^{-1}
T = 100 K
0.35 × 0.10 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.415, T_{max} = 0.863
3802 measured reflections
2090 independent reflections
1776 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.102
S = 1.05
2090 reflections
142 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 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}	0.87 (3)	2.22 (3)	3.021 (2)	153 (2)

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: XU5259).

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