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

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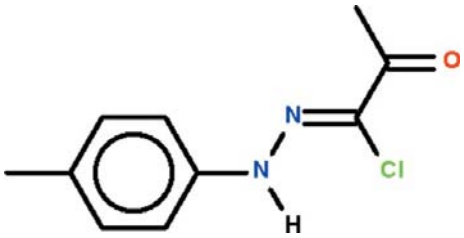
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.045; wR factor = 0.125; data-to-parameter ratio = 10.0.

The asymmetric unit of the title compound, $C_{10}H_{11}ClN_2O$, contains two molecules. The non-H atoms of each molecule lie approximately on a plane (r.m.s. deviations = 0.062 and 0.110 Å), and the C=N double bond has a Z-configuration in both independent molecules. In the crystal, adjacent molecules are linked by $N-H\cdots O_{carbonyl}$ hydrogen bonds, forming chains 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

$C_{10}H_{11}ClN_2O$
M_r = 210.66
Monoclinic, $P2_1$
a = 11.0572 (3) Å
b = 7.6570 (2) Å
c = 12.4613 (3) Å
β = 105.063 (3)°
V = 1018.79 (5) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 3.06 mm^{-1}
T = 100 K
0.20 × 0.02 × 0.02 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.580, T_{max} = 0.941
3467 measured reflections
2667 independent reflections
2516 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.06
2667 reflections
266 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}
Absolute structure: Flack (1983), 533 Friedel pairs
Flack parameter: 0.17 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2	0.88 (5)	2.12 (5)	2.975 (4)	162 (4)
N4—H4···O1^{i}	0.83 (5)	2.12 (5)	2.909 (4)	159 (4)

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

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: XU5262).

References

Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, Oxfordshire, England.
Asiri, A. M., Zayed, M. E. M. & Ng, S. W. (2010). *Acta Cryst.* E**66**, o2374.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Benincori, T., Fusco, R. & Sannicolo, F. (1990). *Gazz. Chim. Ital.* **120**, 635–659.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sayed, S. M., Khalil, M. A., Ahmed, M. A. & Raslan, M. A. (2002). *Synth. Commun.* **32**, 481–495.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.