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

Abdullah M. Asiri,a,b Abdulrahman O. Al-Youbi,a Mohie E. M. Zayeda and Seik Weng Ngc,a*

Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia, b The Center of Excellence for Advanced Materials Research, King Abdul Aziz University, PO Box 8020 Jeddah, Saudi Arabia, and c 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/C27(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, C10H11ClN2O2, 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⋅⋅⋅Ocarbonyl 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

C10H11ClN2O2
M, = 226.66
Monoclinic, P21/c
a = 5.8873 (3) Å

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan
(CrysAlis PRO; Agilent, 2010)
Tmin = 0.415, Tmax = 0.863
3802 measured reflections
2090 independent reflections
1776 reflections with I > 2σ(I)
Rint = 0.026

Refinement

H atoms treated by a mixture of independent and constrained refinement
Δρmax = 0.25 e Å−3
Δρmin = −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+ 0.87 (3) 2.23 (3) 3.02 (2) 153 (2)

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

References