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(*Z*)-2-Sulfanylidene-5-(thiophen-2-ylmethylidene)imidazolidin-4-one

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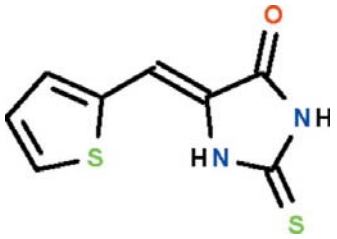
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.043; wR factor = 0.122; data-to-parameter ratio = 12.5.

The molecule of the title compound, $C_8H_6N_2OS_2$, has a V shape with two five-membered rings attached to a methylene C atom. All non-H atoms are approximately coplanar (r.m.s. deviation = 0.096 Å). In the crystal, molecules are linked by N—H···O hydrogen bonds into layers. The thiophene ring is disordered over two positions; the major orientation has an occupancy of 0.683 (3). is there an intramolecular N—H...S bond?

Related literature

For two 5-aryl-2-thioxoimidazolin-4-ones, see: Chowdhry *et al.* (2000); Książek *et al.* (2009).



Experimental

Crystal data

$C_8H_6N_2OS_2$
M_r = 210.27
Triclinic, $P\overline{1}$
a = 6.1022 (6) Å
b = 7.0806 (8) Å
c = 11.0425 (13) Å
α = 72.582 (11)°
β = 76.116 (10)°
γ = 75.640 (9)°
V = 433.87 (8) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 5.22 mm^{-1}
T = 100 K
0.25 × 0.20 × 0.02 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.356, T_{max} = 0.903
2599 measured reflections
1677 independent reflections
1519 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.122
S = 1.04
1677 reflections
134 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 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}	0.88	2.20	2.873 (2)	133

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: BT5612).

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