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2,7-Dimethyl-1,3-thiazolo[4,5-*d*]-pyridazin-4(5*H*)-one

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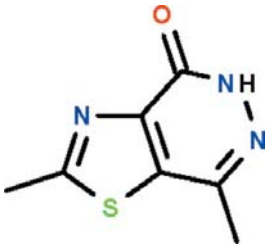
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.029; wR factor = 0.080; data-to-parameter ratio = 13.4.

The nine-membered fused-ring system of the title pyridazine derivative, $C_7H_7N_3OS$, is almost planar (r.m.s. deviation 0.012 Å). In the crystal, the amino H atom forms a hydrogen bond to the ketonic O atom of a neighboring molecule to generate a centrosymmetric dimer.

Related literature

For a related structure, see: Abdel-Aziz *et al.* (2010). For the biological activity of the class of pyridazines, see: Faid-Allah *et al.* (2011); Makki & Faid-Allah (1996).



Experimental

Crystal data

$C_7H_7N_3OS$
M_r = 181.22
Triclinic, $P\overline{1}$
a = 6.9262 (4) Å
b = 7.0540 (4) Å
c = 8.8079 (6) Å
α = 71.002 (6)°
β = 75.845 (5)°
γ = 85.570 (5)°
V = 394.54 (4) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 3.26 mm^{-1}
T = 100 K
0.30 × 0.25 × 0.20 mm

Data collection

Agilent Technologies SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.442, T_{max} = 0.562
2363 measured reflections
1539 independent reflections
1523 reflections with $I > 2\sigma(I)$
R_{int} = 0.012

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.080
S = 1.05
1539 reflections
115 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 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}	0.88 (2)	1.97 (2)	2.845 (2)	173 (2)

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

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: XU5288).

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