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4-(2,7-Dimethyl-4-oxo-1,3-thiazolo[4,5-*d*]-pyridazin-5-yl)benzenesulfonamide

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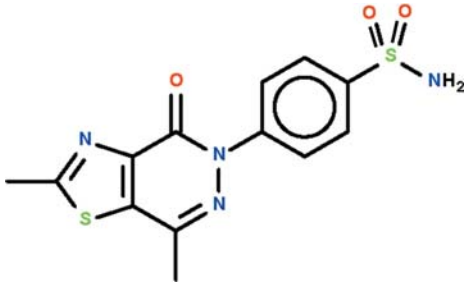
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.097; data-to-parameter ratio = 15.9.

The thiazole–pyridazine fused-ring system of the title compound, $C_{13}H_{12}N_4O_3S_2$, is approximately planar (r.m.s. deviation = 0.037 Å); the benzene ring connected to the fused-ring system through the N atom is twisted by 39.3 (1)°. The amine group uses an H atom to form a hydrogen bond to the ketonic O atom of an inversion-related molecule to generate a dimer; adjacent dimers are linked by an N—H···O hydrogen bond to form a linear chain.

Related literature

For background to related compounds, see: Makki & Faidallah (1996).



Experimental

Crystal data

$C_{13}H_{12}N_4O_3S_2$
M_r = 336.39
Monoclinic, $P2_1/c$
a = 12.6048 (10) Å
b = 13.2273 (10) Å
c = 8.9703 (7) Å
β = 102.242 (1)°
V = 1461.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 100 K
0.20 × 0.15 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.928, T_{max} = 0.945
9962 measured reflections
3333 independent reflections
2888 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.097
S = 1.06
3333 reflections
209 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H1···O1^{i}	0.87 (1)	2.06 (1)	2.922 (2)	169 (2)
N4—H2···O2^{ii}	0.88 (1)	2.38 (2)	3.090 (2)	139 (2)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; 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: XU5226).

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