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2-Ethyl-5*H*-1,3,4-thiadiazolo[3,2-*a*]pyrimidin-5-one

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.096
Data-to-parameter ratio = 13.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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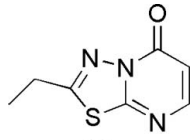
The molecule of the title compound, $C_7H_7N_3OS$, is nearly planar, with a maximum deviation of 0.095 Å from the mean plane for the ethyl group. An intermolecular C—H···O hydrogen bond is observed in the crystal structure.

Comment

The chemistry of thiadiazoles and pyrimidines is well established. The pyrimidine ring is present in several pharmaceutical agents and the thiadiazoles are an important class of chemically and biologically significant compounds. In addition, these nuclei form the active cores of various bioactive molecules (Foroumadi *et al.*, 2005; Farghaly & El-Kashef, 2006). In the light of the above reports and our continued interest in devising new heterocyclic compounds with potential antiviral and antiparasitic activities (da Silva *et al.*, 2005*a*,*b*, 2006), the crystal structure of the title compound, (I), was investigated.



(I)

The molecule of (I) (Fig. 1) is nearly planar, with maximum deviations from the mean plane of −0.094 (2) Å for C6 and 0.095 (2) Å for C7. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). An intermolecular C—H···O hydrogen bond [C—H···O = 2.49 Å] forms a three-dimensional network (Table 1 and Fig. 2).

Experimental

Compound (I) was prepared according to the literature procedure of Cassis *et al.* (1985). Single crystals of (I) suitable for X-ray data collection were obtained by recrystallization from hexane.

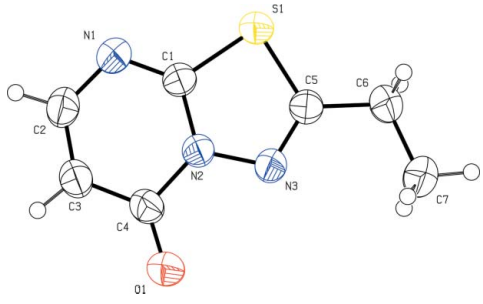


Figure 1
The molecular structure of (I), showing the atom labelling and with displacement ellipsoids drawn at the 50% probability level.

Crystal data

$C_7H_7N_3OS$
M_r = 181.22
Trigonal, $R\overline{3}$
a = 32.347 (5) Å
c = 4.0784 (7) Å
V = 3695.6 (10) Å^3
Z = 18
D_x = 1.466 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 3.13 mm^{-1}
T = 299 (2) K
Prism, colourless
0.48 × 0.30 × 0.28 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2610 measured reflections
1461 independent reflections
1300 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 67.0°
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.096
S = 1.11
1461 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 5.1533P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6A···O1^{i}	0.97	2.49	3.450 (3)	172

Symmetry code: (i) $y+\frac{1}{3}, -x+y+\frac{2}{3}, -z+\frac{8}{3}$.

The H atoms were positioned with idealized geometry, and refined using a riding model, with C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: CAD-4-P; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

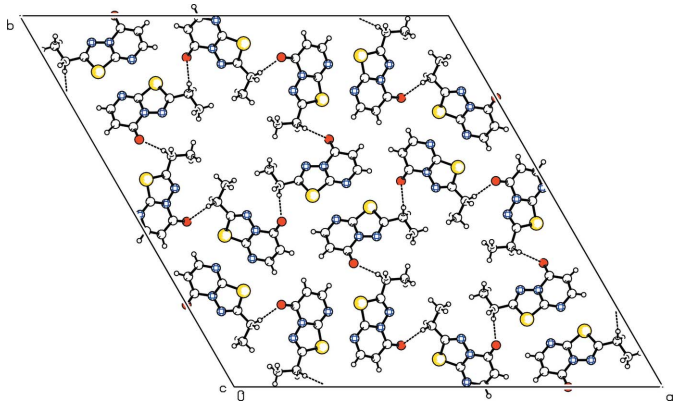


Figure 2
The molecular packing of (I), with hydrogen bonds shown as dashed lines.

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References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Cassis, R., Tapia, R. & Valderrama, J. A. (1985). *Synth. Commun.* **15**, 125–129.
Enraf–Nonius (1996). *CAD-4-PC* . Version 1.2. Enraf–Nonius, Delft, The Netherlands.
Farghaly, A.-R. & El-Kashef, H. (2006). *Arkivoc*, **XI**, 76–90.
Foroumadi, A., Pournourmohammadi, S., Soltani, F., Asgharian-Rezaee, M., Dabiri, S., Kharazmi, A. & Shafiee, A. (2005). *Bioorg. Med. Chem. Lett.* **15**, 1983–1985.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Silva, L. E. da, Joussef, A. C., Foro, S. & Schmidt, B. (2006). *Acta Cryst.* E**62**, o742–o743.
Silva, L. E. da, Joussef, A. C., Nunes, R. J., Andrighetti-Fröhner, C. R. & Bortoluzzi, A. J. (2005*a*). *Acta Cryst.* E**61**, o4121–o4122.
Silva, L. E. da, Joussef, A. C., Nunes, R. J., Andrighetti-Fröhner, C. R. & Bortoluzzi, A. J. (2005*b*). *Acta Cryst.* E**61**, o4252–o4253.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (1987). *REDU4*. Version 6.2c. Stoe & Cie GmbH, Darmstadt, Germany.