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# 3-(2-Ethoxyphenyl)-5-methylsulfanyl-4*H*-1,2,4-triazol-4-amine monohydrate

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**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.044
*wR* factor = 0.114
Data-to-parameter ratio = 13.1

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



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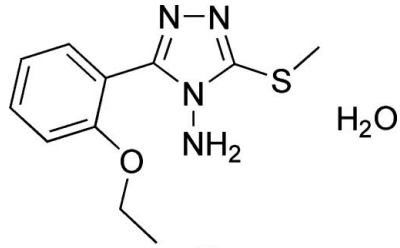
In the title compound, $C_{11}H_{14}N_4OS\cdot H_2O$, the dihedral angle between the ethoxybenzene group and the triazole ring is 48.20 (8)°. Intermolecular N—H···O and O—H···N hydrogen bonds involving the water molecules form a chain along the *a* axis.

## Comment

1,2,4-Triazoles are good intermediates in the synthesis of some fused heterocycles which exhibit various biological properties, including antimicrobial (Feng *et al.*, 1992), antibacterial, anti-fungal (Hui *et al.*, 2002), anti-inflammatory (Prasad *et al.*, 1989) and diuretic (Mohan & Anjaneyulu, 1987) activities.

In the molecule of the title compound, (I) (Fig. 1), the ethoxybenzene fragment (C1–C6/C10/C11/O1) is essentially planar with a maximum deviation of 0.020 (2) Å for atom O1. The dihedral angle between the ethoxybenzene group and the triazole ring is 48.20 (8)°. The C—N bond lengths, in the range 1.304 (3)–1.368 (3) Å, are longer than a typical C=N double bond [*ca* 1.269 (2) Å; Xiang *et al.*, 2004] but shorter than a C—N single bond [*ca* 1.443 (4) Å; Jin *et al.*, 2004], indicating electron delocalization in the triazole ring (Table 1).




(I)

An intramolcular N—H···O hydrogen bond is observed in the main molecule. The crystal packing in (I) (Fig. 2) is stabilized by intermolecular N—H···O and O—H···N hydrogen bonds (Table 2) involving the water molecules. The hydrogen bonds link the molecules into chains along the *a* axis.

## Experimental

Methyl iodide (7.5 mol) and sodium hydroxide (7.0 mol) in dichloromethane (30 ml) were added to 4-amino-5-(2-ethoxyphenyl)-2,4-dihydro[1,2,4]triazole-3-thione (5 mol) at room temperature. The reaction mixture was stirred for 4 h and the white solid obtained was filtered off and recrystallized from a mixture of acetone and petroleum ether (1:2) (yield 68%, m.p. 346–347 K). Single crystals of (I) suitable for X-ray data collection were obtained by slow evaporation of an ethanol solution.

*Crystal data*

$C_{11}H_{14}N_4OS\cdot H_2O$
$M_r = 268.34$
Triclinic, $P\overline{1}$
$a = 7.5828\ (13)$ Å
$b = 8.9824\ (15)$ Å
$c = 11.5308\ (19)$ Å
$\alpha = 109.542\ (3)^\circ$
$\beta = 98.836\ (3)^\circ$
$\gamma = 107.754\ (3)^\circ$
$V = 675.7\ (2)$ Å$^3$
$Z = 2$
$D_x = 1.319$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu = 0.24$ mm$^{-1}$
$T = 298\ (2)$ K
Block, colourless
0.29 × 0.17 × 0.15 mm

*Data collection*

Bruker APEX area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.934$, $T_{max} = 0.960$
3570 measured reflections
2350 independent reflections
2036 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 25.0^\circ$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.114$
$S = 1.04$
2350 reflections
179 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2 + 0.2204P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å$^{-3}$
$\Delta\rho_{min} = -0.27$ e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| S1—C8 | 1.738 (2) | N2—C8 | 1.304 (3) |
| S1—C9 | 1.787 (3) | N3—C8 | 1.355 (2) |
| N1—C7 | 1.304 (3) | N3—C7 | 1.368 (3) |
| N1—N2 | 1.393 (2) | N3—N4 | 1.408 (2) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N4—H4$B$···O2$^{i}$ | 0.876 (17) | 2.129 (18) | 3.004 (3) | 177 (2) |
| N4—H4$A$···O1 | 0.861 (16) | 2.16 (2) | 2.886 (3) | 141 (2) |
| O2—H2$B$···N2$^{ii}$ | 0.852 (16) | 2.065 (16) | 2.894 (2) | 164 (3) |
| O2—H2$A$···N1 | 0.846 (16) | 2.045 (16) | 2.887 (2) | 173 (3) |

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

H atoms bonded to N and O atoms were located in a difference map and were refined using the N—H and O—H distance restraints of 0.86 (2) and 0.85 (2) Å, respectively. The C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of C$sp^2$—H = 0.93 Å with $U_{iso}$(H) = 1.2$U_{eq}$(C), C(methylene)—H = 0.97 Å with $U_{iso}$(H) = 1.2$U_{eq}$(C) and C(methyl)—H = 0.96 Å with $U_{iso}$(H) = 1.5$U_{eq}$(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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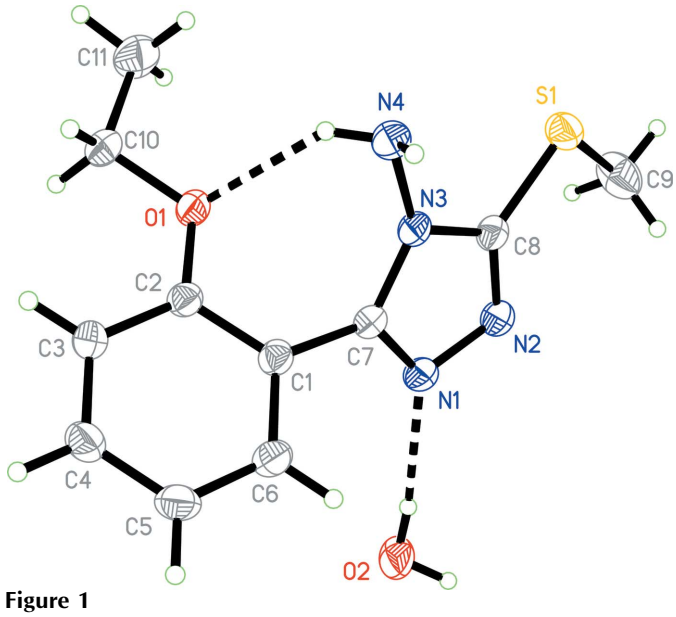


**Figure 1**
The asymmetric unit of (I), with the atom numbering, showing displacement ellipsoids at the 50% probability level. Hydrogen bonds are indicated by dashed lines.

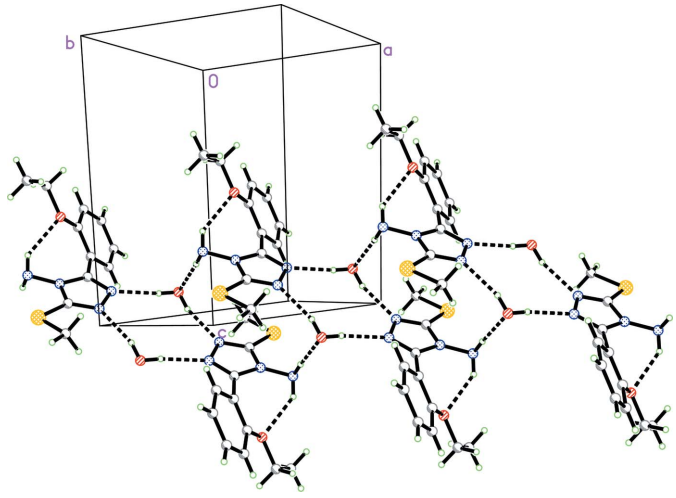


**Figure 2**
Part of the crystal structure of (I), showing a hydrogen-bonded (dashed lines) chain running along the *a* axis.

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