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2-({1-[2-(Methylsulfanyl)phenyl]-1H-tetrazol- 5-yl}sulfanyl)acetic acid

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2-({1-[2-(Methylsulfanyl)phenyl]-1*H*-tetrazol-5-yl}sulfanyl)acetic acid

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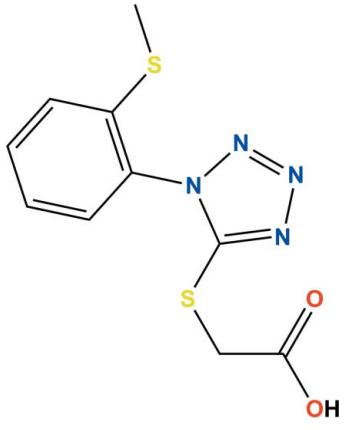
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.004 Å; R factor = 0.051; wR factor = 0.150; data-to-parameter ratio = 14.0.

In the title compound, $C_{10}H_{10}N_4O_2S_2$, the tetrazole and benzene rings are almost normal to one another, with a dihedral angle between their planes of 84.33 (9)°. In the crystal, molecules are linked *via* pairs of bifurcated O—H···(N,N) hydrogen bonds, forming inversion dimers with graph-set motif $R_4^4(12)$. The dimers are linked by significant π–π interactions involving inversion-related tetrazole rings and inversion-related benzene rings, with centroid–centroid distances of 3.7376 (14) and 3.8444 (15) Å, respectively.

Related literature

For details of the ZINC database, see: Irwin *et al.* (2012). For information on the biological properties of tetrazoles, see: Kees *et al.* (1989); Nolte *et al.* (1998); Mafud & Nascimento (2013).



Experimental

Crystal data

$C_{10}H_{10}N_4O_2S_2$
M_r = 282.34
Triclinic, $P\overline{1}$
a = 7.1500 (3) Å
b = 8.3770 (3) Å
c = 11.0890 (5) Å
α = 74.7480 (14)°
β = 79.3090 (14)°
γ = 86.286 (3)°
V = 629.58 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 290 K
0.1 × 0.05 × 0.05 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: for a cylinder mounted on the φ axis (Dwiggins, 1975)
T_{min} = 0.861, T_{max} = 0.862
15888 measured reflections
2335 independent reflections
1879 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.15
S = 1.04
2335 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 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
O1—H1···N1^{i}	0.81 (4)	2.15 (4)	2.952 (4)	176 (4)
O1—H1···N2^{i}	0.81 (4)	2.51 (4)	3.232 (4)	149 (4)

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

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

We are grateful to the CAPES National Council for the Improvement of Higher Education and FAPESP São Paulo Research Foundation for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2571).

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supplementary materials

Acta Cryst. (2013). E**69**, o759 [doi:10.1107/S160053681300980X]

2-({1-[2-(Methylsulfanyl)phenyl]-1*H*-tetrazol-5-yl}sulfanyl)acetic acid

Ana C. Mafud, Yvonne P. Mascarenhas and Alessandro S. Nascimento

Comment

The title acid is a screening molecule available in the ZINC database (Irwin *et al.*, 2012) among the 'drugs-now′ subset. This molecule has been identified as a PPAR gamma ligand candidate in a virtual screening study. The peroxisome proliferator-activated receptors, isoform gamma, are a transcription factors whom regulating the genes expression (Nolte *et al.*, 1998). The binding was further confirmed in experimental binding assays (Mafud *et al.*, 2013). Since tetrazoles are already known to have glucose lowering effects *in vivo* (Kees *et al.*, 1989), in this virtual screening we chose some different representative molecules to evaluate the affinities and the extent of receptor activation. We report herein on the crystal structure of the title compound.

The molecular structure of the title molecule is illustrated in Fig. 1. The tetrazole and phenyl rings are almost normal to one another with a dihedral angle of 84.33 (9)°.

In the crystal, molecules are linked *via* O—H···N hydrogen bonds forming inversion dimers with graph-set motif $R^4_4(12)$; see Fig. 2 and Table 1. The dimers is linked by significant π–π interactions involving inversion related tetrazole rings (*Cg*1 centroid of ring N1—N4/C3) and inversion related phenyl rings (*Cg*2 centroid of ring C4—C9): *Cg*1···*Cg*1^{i} = 3.7376 (14) Å; *Cg*2···*Cg*2^{ii} = 3.8444 (15) Å; symmetry codes: (i) -*x+1*, -*y+1*, -*z*; (ii) -*x+1*, -*y+1*, -*z+1*.

Experimental

A yellow prism-like crystal of the title compound was selected from the sample as supplied (ChemBridge Corporation) without recrystallization.

Refinement

The hydroxyl H atom was located in a difference Fourier map and refined with U_{iso}(H) = 1.5U_{eq}(O). The C-bound H-atoms were included in calculated positions and treated as riding atoms: C—H = 0.93, 0.96 and 0.97 Å, for CH, CH_3 and CH_2 H atoms, respectively, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and = 1.2U_{eq}(C) for other H atoms.

Computing details

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

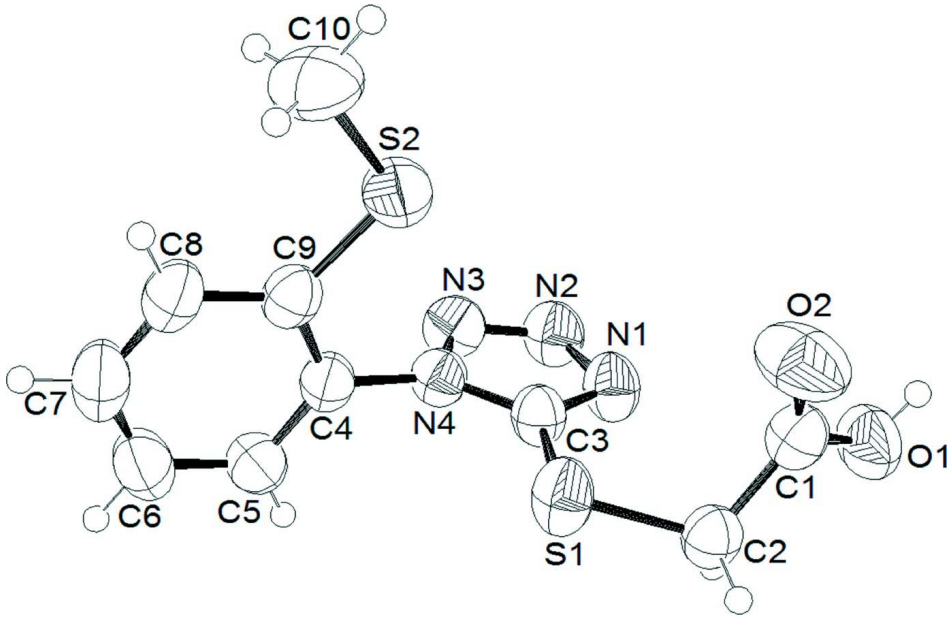

Figure 1

A view of the molecular structure of the title molecule, with atom labelling. The displacement ellipsoids are drawn at the 50% probability level.

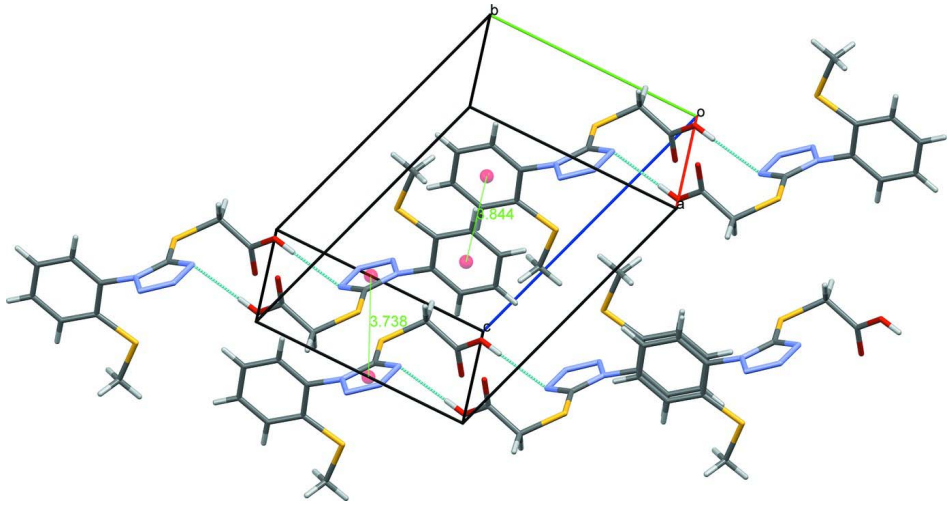

Figure 2

A view of the crystal packing of the title compound, illustrating the O—H···N hydrogen bonds (dashed lines; see Table 1 for details) and the π-π interactions (red ball = ring centroid).

2-({1-[2-(Methylsulfanyl)phenyl]-1*H*-tetrazol-5-yl}sulfanyl)acetic acid

Crystal data

$C_{10}H_{10}N_4O_2S_2$
M_r = 282.34
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.1500 (3) Å
b = 8.3770 (3) Å
c = 11.0890 (5) Å
α = 74.7480 (14)°
β = 79.3090 (14)°
γ = 86.286 (3)°

V = 629.58 (4) Å^3
Z = 2
F(000) = 292
none
D_x = 1.489 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 2086 reflections
θ = 10.4–19.8°
μ = 0.42 mm^{-1}
T = 290 K
Prism, yellow
0.1 × 0.05 × 0.05 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: Fine-focus
Graphite monochromator
CCD scans
Absorption correction: for a cylinder mounted on the φ axis (Dwiggins, 1975)
T_{min} = 0.861, T_{max} = 0.862

15888 measured reflections
2335 independent reflections
1879 reflections with $I > 2\sigma(I)$
R_{int} = 0.079
θ_{max} = 25.7°, θ_{min} = 3.8°
h = −8→8
k = −10→10
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.15
S = 1.04
2335 reflections
167 parameters
0 restraints

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0968P)^2 + 0.1021P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individuallno in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are onlno used when theno are defined bno crnostal snommetrno. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.12427 (8)	0.32835 (9)	0.14822 (6)	0.0644 (3)
S2	0.31586 (12)	0.16473 (8)	0.46904 (6)	0.0744 (3)
O1	0.3263 (3)	0.0525 (3)	−0.07328 (19)	0.0753 (6)
H1	0.367 (6)	−0.039 (5)	−0.072 (4)	0.113*
O2	0.1581 (4)	−0.0338 (3)	0.1185 (2)	0.0973 (8)
N1	0.5089 (3)	0.2791 (3)	0.0763 (2)	0.0593 (5)
N2	0.6701 (3)	0.3173 (3)	0.1112 (2)	0.0621 (5)
N3	0.6313 (3)	0.3917 (3)	0.2004 (2)	0.0593 (5)
N4	0.4384 (2)	0.4047 (2)	0.22640 (17)	0.0490 (4)
C1	0.2079 (3)	0.0747 (3)	0.0282 (2)	0.0576 (6)
C2	0.1398 (3)	0.2518 (3)	0.0096 (2)	0.0546 (5)
H2A	0.0153	0.2615	−0.0148	0.066*
H2B	0.2261	0.3207	−0.0597	0.066*
C3	0.3657 (3)	0.3352 (3)	0.1496 (2)	0.0507 (5)
C4	0.3483 (3)	0.4803 (3)	0.3259 (2)	0.0497 (5)
C5	0.3341 (4)	0.6503 (3)	0.2979 (2)	0.0597 (6)

H5	0.3723	0.7138	0.2153	0.072*
C6	0.2621 (4)	0.7248 (4)	0.3944 (3)	0.0721 (7)
H6	0.2489	0.8394	0.3774	0.087*
C7	0.2099 (4)	0.6277 (4)	0.5165 (3)	0.0736 (8)
H7	0.1645	0.6782	0.5817	0.088*
C8	0.2235 (4)	0.4586 (4)	0.5438 (2)	0.0637 (6)
H8	0.1866	0.396	0.6267	0.076*
C9	0.2925 (3)	0.3800 (3)	0.4476 (2)	0.0539 (5)
C10	0.2427 (5)	0.0824 (4)	0.6350 (3)	0.0923 (10)
H10A	0.3274	0.1185	0.68	0.138*
H10B	0.2456	−0.0363	0.6544	0.138*
H10C	0.1156	0.1204	0.6604	0.138*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0435 (4)	0.0871 (5)	0.0716 (5)	−0.0001 (3)	−0.0027 (3)	−0.0413 (4)
S2	0.0991 (6)	0.0597 (4)	0.0580 (4)	−0.0016 (3)	−0.0056 (3)	−0.0094 (3)
O1	0.0897 (14)	0.0694 (12)	0.0682 (12)	0.0092 (10)	−0.0035 (10)	−0.0296 (10)
O2	0.1136 (18)	0.0716 (13)	0.0805 (14)	0.0116 (12)	0.0131 (12)	0.0020 (11)
N1	0.0483 (10)	0.0683 (12)	0.0648 (12)	−0.0004 (9)	0.0007 (8)	−0.0307 (10)
N2	0.0473 (10)	0.0726 (13)	0.0670 (13)	0.0032 (9)	−0.0015 (9)	−0.0260 (11)
N3	0.0434 (10)	0.0711 (13)	0.0628 (12)	0.0002 (8)	−0.0052 (8)	−0.0192 (10)
N4	0.0425 (9)	0.0543 (10)	0.0501 (10)	0.0014 (7)	−0.0045 (7)	−0.0163 (8)
C1	0.0544 (12)	0.0648 (14)	0.0558 (14)	−0.0015 (10)	−0.0109 (10)	−0.0186 (11)
C2	0.0496 (12)	0.0600 (13)	0.0571 (13)	−0.0012 (10)	−0.0111 (10)	−0.0188 (11)
C3	0.0475 (11)	0.0545 (12)	0.0522 (12)	0.0008 (9)	−0.0048 (9)	−0.0205 (10)
C4	0.0460 (11)	0.0569 (12)	0.0506 (12)	0.0024 (9)	−0.0103 (9)	−0.0206 (10)
C5	0.0611 (14)	0.0563 (14)	0.0640 (14)	0.0032 (10)	−0.0140 (11)	−0.0184 (11)
C6	0.0711 (16)	0.0646 (16)	0.094 (2)	0.0088 (12)	−0.0231 (14)	−0.0392 (15)
C7	0.0624 (15)	0.095 (2)	0.0812 (19)	0.0070 (14)	−0.0154 (13)	−0.0530 (17)
C8	0.0594 (14)	0.0837 (18)	0.0538 (13)	0.0016 (12)	−0.0090 (10)	−0.0289 (12)
C9	0.0481 (11)	0.0649 (14)	0.0514 (12)	0.0001 (10)	−0.0096 (9)	−0.0193 (10)
C10	0.096 (2)	0.093 (2)	0.0671 (18)	0.0006 (17)	−0.0007 (15)	0.0068 (16)

Geometric parameters (Å, º)

S1—C3	1.734 (2)	C2—H2B	0.97
S1—C2	1.798 (2)	C4—C5	1.376 (3)
S2—C9	1.757 (3)	C4—C9	1.391 (3)
S2—C10	1.778 (3)	C5—C6	1.381 (4)
O1—C1	1.324 (3)	C5—H5	0.93
O1—H1	0.80 (4)	C6—C7	1.380 (4)
O2—C1	1.177 (3)	C6—H6	0.93
N1—C3	1.327 (3)	C7—C8	1.369 (4)
N1—N2	1.364 (3)	C7—H7	0.93
N2—N3	1.282 (3)	C8—C9	1.395 (3)
N3—N4	1.359 (3)	C8—H8	0.93
N4—C3	1.341 (3)	C10—H10A	0.96
N4—C4	1.444 (3)	C10—H10B	0.96

C1—C2	1.504 (3)	C10—H10C	0.96
C2—H2A	0.97		
C3—S1—C2	98.45 (10)	C9—C4—N4	118.91 (19)
C9—S2—C10	104.17 (14)	C4—C5—C6	118.8 (2)
C1—O1—H1	118 (3)	C4—C5—H5	120.6
C3—N1—N2	105.52 (19)	C6—C5—H5	120.6
N3—N2—N1	111.51 (18)	C7—C6—C5	119.3 (3)
N2—N3—N4	106.22 (18)	C7—C6—H6	120.3
C3—N4—N3	108.48 (17)	C5—C6—H6	120.3
C3—N4—C4	131.62 (18)	C8—C7—C6	121.6 (2)
N3—N4—C4	119.88 (18)	C8—C7—H7	119.2
O2—C1—O1	123.2 (2)	C6—C7—H7	119.2
O2—C1—C2	125.3 (2)	C7—C8—C9	120.2 (2)
O1—C1—C2	111.4 (2)	C7—C8—H8	119.9
C1—C2—S1	113.73 (17)	C9—C8—H8	119.9
C1—C2—H2A	108.8	C4—C9—C8	117.2 (2)
S1—C2—H2A	108.8	C4—C9—S2	117.76 (17)
C1—C2—H2B	108.8	C8—C9—S2	125.01 (19)
S1—C2—H2B	108.8	S2—C10—H10A	109.5
H2A—C2—H2B	107.7	S2—C10—H10B	109.5
N1—C3—N4	108.27 (19)	H10A—C10—H10B	109.5
N1—C3—S1	127.70 (17)	S2—C10—H10C	109.5
N4—C3—S1	124.01 (16)	H10A—C10—H10C	109.5
C5—C4—C9	122.8 (2)	H10B—C10—H10C	109.5
C5—C4—N4	118.2 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.81 (4)	2.15 (4)	2.952 (4)	176 (4)
O1—H1···N2^{i}	0.81 (4)	2.51 (4)	3.232 (4)	149 (4)

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