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2-Methylsulfanyl-1,2,4-triazolo[1,5-*a*]-quinazolin-5(4*H*)-one

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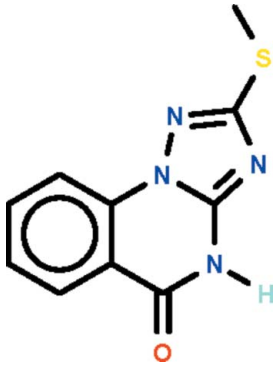
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.089; data-to-parameter ratio = 13.6.

The non-H atoms of the title compound, $C_{10}H_8N_4OS$, lie approximately in a common plane (r.m.s. deviation = 0.058 Å). In the crystal, two molecules are linked across a center of inversion by a pair of N—H···N hydrogen bonds, forming a a dimer.

Related literature

For the synthesis, see: Al-Salahi & Geffken (2011). For a related compound, see: Al-Salahi *et al.* (2011).



Experimental

Crystal data

$C_{10}H_8N_4OS$ M_r = 232.26
Monoclinic, $P2_1/c$
a = 10.4150 (1) Å
b = 5.0631 (1) Å
c = 18.6564 (3) Å
β = 96.857 (1)°
V = 976.76 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.81 mm^{-1}
T = 294 K
0.35 × 0.15 × 0.10 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.439, T_{max} = 0.766
15980 measured reflections
2052 independent reflections
1996 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.089
S = 1.05
2052 reflections
151 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···N3^{i}	0.85 (2)	2.05 (2)	2.896 (2)	174 (2)

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

Data collection: *CrysAlis PRO* (Agilent, 2012); 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: BT5914).

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supporting information

Acta Cryst. (2012). E**68**, o1805 [doi:10.1107/S1600536812021757]

2-Methylsulfanyl-1,2,4-triazolo[1,5-*a*]quinazolin-5(4*H*)-one

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S1. Comment

The title compound (Scheme I) was synthesized from 2-hydrazinobenzoic acid and dimethyl *N*-cyanoimidodithiocarbonate; further reactions on the inherent lactam unit yielded other derivatives (Al-Salahi & Geffken, 2011). The non-H atoms of $C_{10}H_8N_4OS$ lie in a common plane (Fig. 1). Two molecules are linked across a center-of-inversion by N–H···N hydrogen bonds to form a dimer (Table 1). A related compound that has a benzyloxy group instead of the methylsulfanyl group also exists as a hydrogen-bonded dimer (Al-Salahi *et al.*, 2011).

S2. Experimental

Under ice-cold conditions, 2-hydrazinobenzoic acid (10 mmol, 1.52 g) was added to a solution of dimethyl *N*-cyanodithioimidocarbonate (10 mmol, 1.46 g) in ethanol (20 ml). Triethylamine (30 mmol, 3.03 g) was added. The reaction mixture was stirred overnight at room temperature. Concentrated hydrochloric acid was added; the acidified mixture for heated for an hour. The mixture was poured into ice water; the solid that formed was collected and recrystallized from ethanol to give colorless crystals.

S3. Refinement

All H-atom were located in a difference Fourier map. Carbon-bound H-atoms were placed in calculated positions [C–H 0.93 to 0.96 Å, U_{iso}(H) 1.2 to 1.5U_{eq}(C)] and were included in the refinement in the riding model approximation.

The amino H-atom was freely refined.

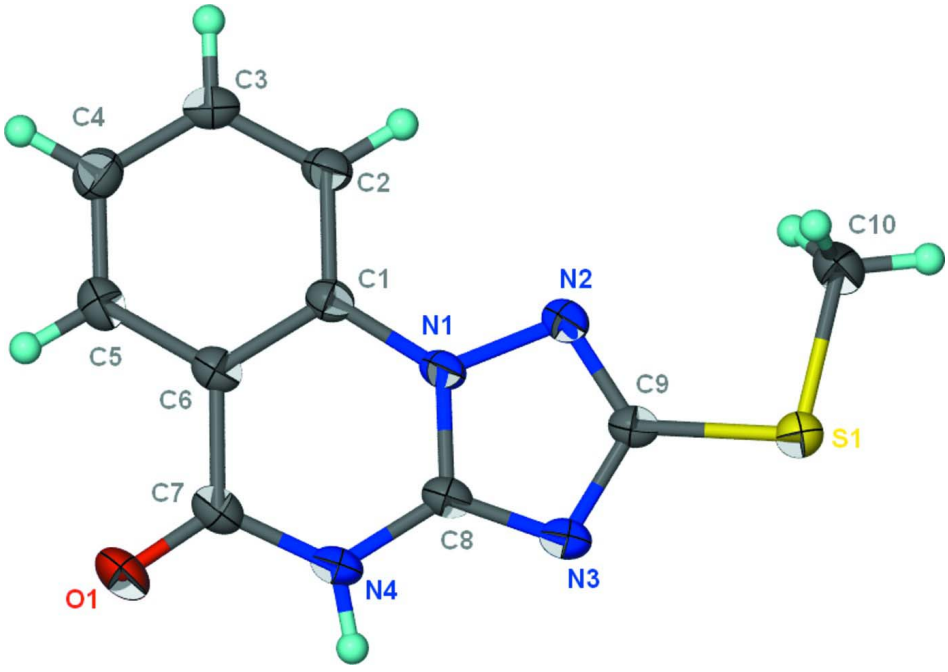

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{10}H_8N_4OS$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-Methylsulfanyl-1,2,4-triazolo[1,5-*a*]quinazolin-5(4*H*)-one

Crystal data

$C_{10}H_8N_4OS$
$M_r = 232.26$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.4150$ (1) Å
$b = 5.0631$ (1) Å
$c = 18.6564$ (3) Å
$\beta = 96.857$ (1)°
$V = 976.76$ (3) Å^3
$Z = 4$
$F(000) = 480$
$D_x = 1.579$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 10679 reflections
$\theta = 4.3$–$76.7°$
$\mu = 2.81$ mm^{-1}
$T = 294$ K
Prism, colorless
0.35 × 0.15 × 0.10 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min} = 0.439$, $T_{max} = 0.766$
15980 measured reflections
2052 independent reflections
1996 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 76.9°$, $\theta_{min} = 4.3°$
$h = -13 \rightarrow 13$
$k = -6 \rightarrow 6$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.089$
$S = 1.05$
2052 reflections
151 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.2828P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0089 (9)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.07695 (3)	0.09449 (7)	0.203762 (17)	0.03356 (15)
O1	0.19589 (12)	1.1102 (2)	−0.05498 (6)	0.0527 (3)
N1	0.25468 (10)	0.6522 (2)	0.12100 (5)	0.0284 (2)
N2	0.24857 (10)	0.4808 (2)	0.17833 (5)	0.0299 (2)
N3	0.07817 (11)	0.4211 (2)	0.09036 (6)	0.0327 (3)
N4	0.13609 (11)	0.7645 (3)	0.01027 (6)	0.0365 (3)
C1	0.34851 (12)	0.8433 (3)	0.11483 (6)	0.0282 (3)
C2	0.45835 (13)	0.8685 (3)	0.16496 (7)	0.0331 (3)
H2	0.4716	0.7559	0.2045	0.040*
C3	0.54687 (13)	1.0631 (3)	0.15483 (8)	0.0357 (3)
H3	0.6209	1.0803	0.1877	0.043*
C4	0.52720 (14)	1.2342 (3)	0.09627 (8)	0.0381 (3)
H4A	0.5867	1.3674	0.0908	0.046*
C5	0.41916 (13)	1.2058 (3)	0.04634 (7)	0.0365 (3)
H5	0.4066	1.3195	0.0070	0.044*
C6	0.32892 (12)	1.0088 (3)	0.05434 (7)	0.0311 (3)
C7	0.21660 (14)	0.9725 (3)	−0.00156 (7)	0.0359 (3)
C8	0.15228 (12)	0.6134 (3)	0.07104 (7)	0.0303 (3)
C9	0.14125 (12)	0.3490 (3)	0.15648 (7)	0.0291 (3)
C10	0.18994 (15)	0.0881 (3)	0.28453 (8)	0.0443 (4)
H10A	0.1713	−0.0598	0.3138	0.066*
H10B	0.1826	0.2487	0.3111	0.066*
H10C	0.2763	0.0721	0.2718	0.066*
H4	0.072 (2)	0.722 (4)	−0.0199 (11)	0.062 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0327 (2)	0.0351 (2)	0.0319 (2)	−0.00273 (12)	−0.00017 (14)	0.00156 (12)
O1	0.0552 (7)	0.0637 (8)	0.0356 (6)	−0.0047 (5)	−0.0093 (5)	0.0204 (5)
N1	0.0297 (5)	0.0316 (5)	0.0225 (5)	0.0011 (4)	−0.0028 (4)	0.0021 (4)
N2	0.0315 (5)	0.0323 (6)	0.0249 (5)	0.0010 (4)	−0.0010 (4)	0.0025 (4)

N3	0.0308 (5)	0.0381 (6)	0.0273 (5)	−0.0004 (4)	−0.0038 (4)	0.0003 (4)
N4	0.0364 (6)	0.0439 (7)	0.0263 (5)	−0.0022 (5)	−0.0087 (4)	0.0045 (5)
C1	0.0298 (6)	0.0300 (6)	0.0246 (6)	0.0029 (5)	0.0018 (5)	−0.0023 (5)
C2	0.0345 (6)	0.0356 (7)	0.0275 (6)	0.0012 (5)	−0.0031 (5)	0.0007 (5)
C3	0.0328 (6)	0.0399 (7)	0.0328 (7)	−0.0007 (5)	−0.0020 (5)	−0.0048 (5)
C4	0.0394 (7)	0.0364 (7)	0.0387 (7)	−0.0050 (6)	0.0051 (6)	−0.0020 (6)
C5	0.0428 (7)	0.0356 (7)	0.0312 (7)	0.0012 (6)	0.0049 (6)	0.0046 (5)
C6	0.0335 (6)	0.0335 (7)	0.0258 (6)	0.0039 (5)	0.0015 (5)	0.0000 (5)
C7	0.0385 (7)	0.0413 (7)	0.0269 (6)	0.0034 (6)	−0.0008 (5)	0.0035 (6)
C8	0.0310 (6)	0.0340 (7)	0.0245 (6)	0.0030 (5)	−0.0029 (5)	−0.0009 (5)
C9	0.0291 (6)	0.0314 (6)	0.0260 (6)	0.0027 (5)	0.0000 (5)	−0.0023 (5)
C10	0.0442 (8)	0.0510 (9)	0.0354 (7)	−0.0051 (6)	−0.0041 (6)	0.0098 (6)

Geometric parameters (Å, º)

S1—C9	1.7402 (14)	C1—C6	1.4008 (18)
S1—C10	1.7980 (15)	C2—C3	1.378 (2)
O1—C7	1.2145 (18)	C2—H2	0.9300
N1—C8	1.3443 (15)	C3—C4	1.390 (2)
N1—N2	1.3848 (15)	C3—H3	0.9300
N1—C1	1.3897 (17)	C4—C5	1.3800 (19)
N2—C9	1.3237 (17)	C4—H4A	0.9300
N3—C8	1.3192 (18)	C5—C6	1.391 (2)
N3—C9	1.3759 (16)	C5—H5	0.9300
N4—C8	1.3614 (17)	C6—C7	1.4828 (18)
N4—C7	1.3800 (19)	C10—H10A	0.9600
N4—H4	0.85 (2)	C10—H10B	0.9600
C1—C2	1.3942 (17)	C10—H10C	0.9600
C9—S1—C10	100.67 (7)	C4—C5—C6	120.60 (13)
C8—N1—N2	109.76 (10)	C4—C5—H5	119.7
C8—N1—C1	123.49 (11)	C6—C5—H5	119.7
N2—N1—C1	126.72 (10)	C5—C6—C1	118.70 (12)
C9—N2—N1	101.13 (10)	C5—C6—C7	120.00 (12)
C8—N3—C9	102.03 (11)	C1—C6—C7	121.28 (13)
C8—N4—C7	123.00 (11)	O1—C7—N4	121.17 (13)
C8—N4—H4	114.7 (15)	O1—C7—C6	123.63 (14)
C7—N4—H4	122.3 (15)	N4—C7—C6	115.18 (12)
N1—C1—C2	122.47 (12)	N3—C8—N1	111.11 (11)
N1—C1—C6	116.55 (11)	N3—C8—N4	128.60 (11)
C2—C1—C6	120.97 (12)	N1—C8—N4	120.29 (12)
C3—C2—C1	118.83 (13)	N2—C9—N3	115.95 (12)
C3—C2—H2	120.6	N2—C9—S1	125.39 (9)
C1—C2—H2	120.6	N3—C9—S1	118.65 (10)
C2—C3—C4	121.01 (13)	S1—C10—H10A	109.5
C2—C3—H3	119.5	S1—C10—H10B	109.5
C4—C3—H3	119.5	H10A—C10—H10B	109.5
C5—C4—C3	119.85 (13)	S1—C10—H10C	109.5

C5—C4—H4A	120.1	H10A—C10—H10C	109.5
C3—C4—H4A	120.1	H10B—C10—H10C	109.5
C8—N1—N2—C9	0.85 (13)	C5—C6—C7—O1	−1.4 (2)
C1—N1—N2—C9	179.10 (12)	C1—C6—C7—O1	−179.72 (14)
C8—N1—C1—C2	−175.64 (12)	C5—C6—C7—N4	177.42 (13)
N2—N1—C1—C2	6.33 (19)	C1—C6—C7—N4	−0.88 (19)
C8—N1—C1—C6	3.12 (18)	C9—N3—C8—N1	1.23 (14)
N2—N1—C1—C6	−174.91 (11)	C9—N3—C8—N4	−178.64 (14)
N1—C1—C2—C3	179.92 (12)	N2—N1—C8—N3	−1.39 (15)
C6—C1—C2—C3	1.2 (2)	C1—N1—C8—N3	−179.71 (11)
C1—C2—C3—C4	0.7 (2)	N2—N1—C8—N4	178.50 (11)
C2—C3—C4—C5	−1.6 (2)	C1—N1—C8—N4	0.17 (19)
C3—C4—C5—C6	0.6 (2)	C7—N4—C8—N3	175.64 (14)
C4—C5—C6—C1	1.3 (2)	C7—N4—C8—N1	−4.2 (2)
C4—C5—C6—C7	−177.05 (13)	N1—N2—C9—N3	−0.07 (14)
N1—C1—C6—C5	179.03 (12)	N1—N2—C9—S1	179.08 (9)
C2—C1—C6—C5	−2.2 (2)	C8—N3—C9—N2	−0.71 (15)
N1—C1—C6—C7	−2.66 (18)	C8—N3—C9—S1	−179.93 (9)
C2—C1—C6—C7	176.13 (12)	C10—S1—C9—N2	2.50 (13)
C8—N4—C7—O1	−176.73 (14)	C10—S1—C9—N3	−178.36 (11)
C8—N4—C7—C6	4.4 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···N3^{i}	0.85 (2)	2.05 (2)	2.896 (2)	174 (2)

Symmetry code: (i) −*x*, −*y*+1, −*z*.