Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Propyl-4*H*-thiazolo[3,2-*a*][1,3,5]-triazine-4-thione

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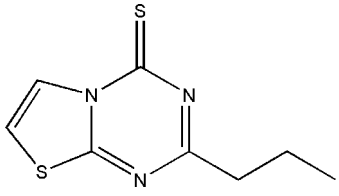
Received 27 February 2008; accepted 11 March 2008

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.024; wR factor = 0.069; data-to-parameter ratio = 14.0.

In the title compound, $C_8H_9N_3S_2$, the *n*-propyl chain is disordered over two orientations (site-occupancy ratio = 0.522:0.478) and is roughly perpendicular to the fused thiazolotriazine system. The angle between the fused ring and the propyl chain is 83.6 (1)° [82.2 (1)° for the disordered chain]. The structure is stabilized by C—H···N hydrogen bonds.

Related literature

For related literature, see: Jiang *et al.* (2007); Pauling *et al.* (1960); Yunus *et al.* (2007).



Experimental

Crystal data

$C_8H_9N_3S_2$
M_r = 211.32
Monoclinic, $P2_1/c$
a = 9.3240 (7) Å
b = 14.9973 (11) Å
c = 6.8063 (5) Å
β = 95.505 (1)°
V = 947.37 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.52 mm^{-1}
T = 173 (2) K
0.32 × 0.25 × 0.22 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.853, T_{max} = 0.895
5571 measured reflections
2254 independent reflections
2077 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.068
S = 1.05
2254 reflections
161 parameters
5 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···N2^{i}	0.95	2.38	3.3261 (16)	171

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors gratefully acknowledge Allama Iqbal Open University, Islamabad, Pakistan, for providing research facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2086).

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supporting information

Acta Cryst. (2008). E**64**, o722 [doi:10.1107/S1600536808006752]

2-Propyl-4*H*-thiazolo[3,2-*a*][1,3,5]triazine-4-thione

Uzma Yunus, Muhammad Kalim Tahir, Moazzam Hussain Bhatti and Wai-Yeung Wong

S1. Comment

We have previously reported the crystal structure of 2-phenyl-4*H*-thiazolo[3,2,-a]- [1,3,5]triazine-4-thione with a phenyl group attached to the 1,3,5-triazine ring (Yunus *et al.*, 2007). The molecule was essentially planar. In contrast, in the title compound the pendant *n*-propyl group is almost perpendicular to the fused thiazolo[3,2,-a][1,3,5]triazine ring, which are themselves co-planar (maximum deviation from mean plane is 0.0437 (1) Å from atom C4). The *n*-propyl chain is disordered over two orientations with a site occupancy ratio of 0.522:0.478 (Jiang *et al.*, 2007). The CN bond distances of the 1,3,5-triazine ring are in the range 1.3191 (15) to 1.4093 (14) Å, in which N1—C5 bond length is slightly longer than that of N2—C5. These values are intermediate between those expected for single and double C—N bonds (1.47 and 1.27 Å, respectively). The C=S bond length of 1.6686 (12) Å is similar to that of the phenyl analog (Yunus *et al.*, 2007) but is slightly longer then the pure double bond distance (1.61 Å) (Pauling 1960). The bond angles and bond lengths in the thiazole ring are within the normal ranges. The crystal structure is stabilized by weak C—H···N hydrogen bonding interactions.

S2. Experimental

A mixture of ammonium thiocyanate (26 mmol) and butyryl chloride (26 mmol) in dry acetone (60 ml) was stirred for 30 min. Then 2-aminothiazole (26 mmol) was added and the reaction mixture was refluxed for 2 h. After cooling, the reaction mixture was poured into acidified cold water. The resulting yellow solid was filtered and washed with cold acetone. Single crystals of the title compound suitable for single-crystal *x*-ray analysis were obtained by recrystallization of the yellow solid from acetonitrile.

S3. Refinement

H atoms were found in difference Fourier maps and subsequently placed in idealized positions with constrained C—H distances of 0.98 Å (RCH_3), 0.99 Å (R_2CH_2) and 0.95 Å ($C_{Ar}H$) with U_{iso}(H) values set to either $1.5U_{eq}$ (RCH_3) or $1.2U_{eq}$ of the attached C atom.

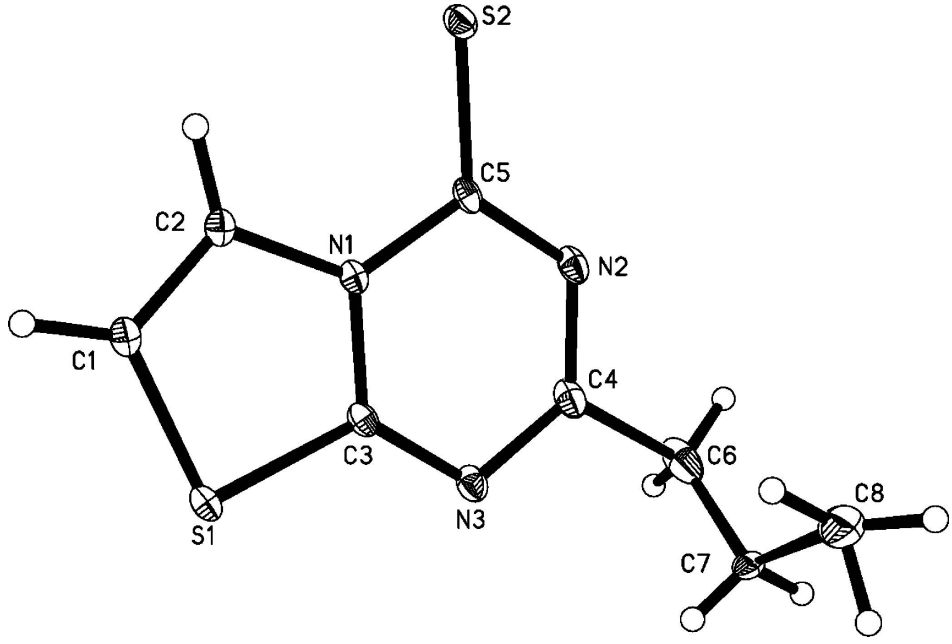

Figure 1

A view of the molecular structure. Displacement ellipsoids are drawn at the 50% probability level.

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$\beta = 95.505\ (1)°$
$V = 947.37\ (12)$ Å^3
$Z = 4$
$F(000) = 440$
$D_x = 1.481$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5571 reflections
$\theta = 2.6–28.3°$
$\mu = 0.52$ mm^{-1}
$T = 173$ K
Block, pale yellow
0.32 × 0.25 × 0.22 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{min} = 0.853$, $T_{max} = 0.895$
5571 measured reflections
2254 independent reflections
2077 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.6°$
$h = -12\rightarrow12$
$k = -19\rightarrow14$
$l = -9\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.068$
$S = 1.05$
2254 reflections
161 parameters
5 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0392P)^2 + 0.2601P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0066 (12)

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 individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.20093 (3)	0.710163 (18)	0.27470 (4)	0.02095 (10)	
S2	−0.15462 (3)	0.443002 (19)	0.21702 (4)	0.02265 (10)	
N1	0.04853 (10)	0.56884 (6)	0.25767 (13)	0.01739 (19)	
N2	0.12868 (11)	0.42185 (7)	0.29852 (15)	0.0235 (2)	
N3	0.29929 (11)	0.54164 (7)	0.31895 (15)	0.0231 (2)	
C1	0.01557 (13)	0.71890 (8)	0.23196 (17)	0.0224 (2)	
H1	−0.0344	0.7739	0.2143	0.027*	
C2	−0.04951 (12)	0.63902 (8)	0.22664 (17)	0.0211 (2)	
H2	−0.1508	0.6311	0.2043	0.025*	
C3	0.18861 (12)	0.59613 (7)	0.28536 (15)	0.0185 (2)	
C5	0.01588 (12)	0.47711 (7)	0.25939 (15)	0.0187 (2)	
C4	0.26174 (14)	0.45502 (8)	0.32834 (18)	0.0259 (3)	0.522 (4)
C6	0.3713 (6)	0.3883 (4)	0.4050 (7)	0.0221 (9)	0.522 (4)
H6A	0.3288	0.3278	0.4003	0.029 (8)*	0.522 (4)
H6B	0.4062	0.4022	0.5436	0.025 (7)*	0.522 (4)
C7	0.4958 (2)	0.39267 (16)	0.2751 (4)	0.0248 (6)	0.522 (4)
H7A	0.5357	0.4539	0.2799	0.021 (7)*	0.522 (4)
H7B	0.5730	0.3517	0.3292	0.036 (8)*	0.522 (4)
C8	0.4516 (9)	0.3679 (6)	0.0614 (6)	0.0357 (13)	0.522 (4)
H8A	0.5357	0.3714	−0.0143	0.030 (8)*	0.522 (4)
H8B	0.3773	0.4093	0.0055	0.045 (10)*	0.522 (4)
H8C	0.4134	0.3070	0.0552	0.061 (12)*	0.522 (4)
C4A	0.26174 (14)	0.45502 (8)	0.32834 (18)	0.0259 (3)	0.478 (4)
C6A	0.3938 (7)	0.3911 (4)	0.3487 (8)	0.0255 (12)	0.478 (4)
H6A1	0.4827	0.4276	0.3621	0.047 (11)*	0.478 (4)
H6A2	0.3913	0.3565	0.4722	0.038 (11)*	0.478 (4)
C7A	0.4034 (3)	0.32554 (16)	0.1781 (4)	0.0247 (7)	0.478 (4)
H7A1	0.4736	0.2781	0.2199	0.036 (9)*	0.478 (4)
H7A2	0.3083	0.2970	0.1461	0.037 (9)*	0.478 (4)

C8A	0.4491 (8)	0.3709 (6)	−0.0056 (8)	0.0320 (11)	0.478 (4)
H8A1	0.4583	0.3263	−0.1087	0.064 (14)*	0.478 (4)
H8A2	0.5420	0.4007	0.0263	0.061 (13)*	0.478 (4)
H8A3	0.3764	0.4152	−0.0528	0.030 (9)*	0.478 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02618 (16)	0.01417 (15)	0.02233 (16)	−0.00294 (10)	0.00150 (11)	0.00001 (9)
S2	0.02469 (16)	0.01845 (15)	0.02542 (16)	−0.00432 (10)	0.00559 (11)	−0.00188 (10)
N1	0.0225 (4)	0.0139 (4)	0.0155 (4)	−0.0004 (3)	0.0008 (3)	0.0001 (3)
N2	0.0307 (5)	0.0151 (4)	0.0231 (5)	0.0010 (4)	−0.0059 (4)	−0.0003 (4)
N3	0.0254 (5)	0.0183 (5)	0.0243 (5)	0.0009 (4)	−0.0051 (4)	−0.0020 (4)
C1	0.0273 (6)	0.0166 (5)	0.0236 (6)	0.0020 (4)	0.0037 (4)	−0.0001 (4)
C2	0.0235 (5)	0.0172 (5)	0.0226 (5)	0.0024 (4)	0.0029 (4)	0.0003 (4)
C3	0.0247 (5)	0.0157 (5)	0.0147 (5)	−0.0022 (4)	0.0000 (4)	−0.0010 (4)
C5	0.0280 (5)	0.0148 (5)	0.0130 (5)	−0.0015 (4)	0.0010 (4)	−0.0015 (4)
C4	0.0301 (6)	0.0183 (5)	0.0266 (6)	0.0025 (4)	−0.0106 (5)	−0.0023 (4)
C6	0.0217 (16)	0.0211 (14)	0.023 (2)	0.0022 (11)	−0.0009 (16)	0.0060 (18)
C7	0.0159 (11)	0.0253 (12)	0.0332 (13)	0.0029 (8)	0.0023 (9)	−0.0008 (9)
C8	0.0347 (17)	0.039 (2)	0.034 (3)	0.0051 (15)	0.006 (3)	−0.009 (3)
C4A	0.0301 (6)	0.0183 (5)	0.0266 (6)	0.0025 (4)	−0.0106 (5)	−0.0023 (4)
C6A	0.032 (3)	0.0196 (16)	0.023 (3)	0.0051 (16)	−0.0085 (19)	0.0019 (19)
C7A	0.0224 (11)	0.0180 (12)	0.0337 (15)	0.0042 (9)	0.0030 (10)	0.0003 (10)
C8A	0.0268 (16)	0.0325 (18)	0.038 (3)	−0.0014 (13)	0.009 (3)	0.004 (3)

Geometric parameters (Å, º)

S1—C3	1.7161 (11)	C6—H6B	0.9900
S1—C1	1.7299 (13)	C7—C8	1.519 (5)
S2—C5	1.6686 (12)	C7—H7A	0.9900
N1—C3	1.3644 (14)	C7—H7B	0.9900
N1—C2	1.3967 (14)	C8—H8A	0.9800
N1—C5	1.4093 (14)	C8—H8B	0.9800
N2—C4	1.3340 (16)	C8—H8C	0.9800
N2—C5	1.3455 (15)	C6A—C7A	1.531 (6)
N3—C3	1.3191 (15)	C6A—H6A1	0.9900
N3—C4	1.3485 (15)	C6A—H6A2	0.9900
C1—C2	1.3418 (17)	C7A—C8A	1.520 (6)
C1—H1	0.9500	C7A—H7A1	0.9900
C2—H2	0.9500	C7A—H7A2	0.9900
C4—C6	1.488 (6)	C8A—H8A1	0.9800
C6—C7	1.526 (5)	C8A—H8A2	0.9800
C6—H6A	0.9900	C8A—H8A3	0.9800
C3—S1—C1	90.73 (6)	C8—C7—C6	113.1 (4)
C3—N1—C2	113.50 (9)	C8—C7—H7A	109.0
C3—N1—C5	119.76 (9)	C6—C7—H7A	109.0

C2—N1—C5	126.73 (10)	C8—C7—H7B	109.0
C4—N2—C5	119.89 (10)	C6—C7—H7B	109.0
C3—N3—C4	113.74 (10)	H7A—C7—H7B	107.8
C2—C1—S1	112.26 (9)	C7—C8—H8A	109.5
C2—C1—H1	123.9	C7—C8—H8B	109.5
S1—C1—H1	123.9	H8A—C8—H8B	109.5
C1—C2—N1	112.39 (10)	C7—C8—H8C	109.5
C1—C2—H2	123.8	H8A—C8—H8C	109.5
N1—C2—H2	123.8	H8B—C8—H8C	109.5
N3—C3—N1	124.11 (10)	C7A—C6A—H6A1	108.4
N3—C3—S1	124.77 (9)	C7A—C6A—H6A2	108.4
N1—C3—S1	111.11 (8)	H6A1—C6A—H6A2	107.5
N2—C5—N1	115.95 (10)	C8A—C7A—C6A	112.2 (4)
N2—C5—S2	123.99 (9)	C8A—C7A—H7A1	109.2
N1—C5—S2	120.05 (8)	C6A—C7A—H7A1	109.2
N2—C4—N3	126.44 (11)	C8A—C7A—H7A2	109.2
N2—C4—C6	113.6 (3)	C6A—C7A—H7A2	109.2
N3—C4—C6	119.4 (3)	H7A1—C7A—H7A2	107.9
C4—C6—C7	107.7 (3)	C7A—C8A—H8A1	109.5
C4—C6—H6A	110.2	C7A—C8A—H8A2	109.5
C7—C6—H6A	110.2	H8A1—C8A—H8A2	109.5
C4—C6—H6B	110.2	C7A—C8A—H8A3	109.5
C7—C6—H6B	110.2	H8A1—C8A—H8A3	109.5
H6A—C6—H6B	108.5	H8A2—C8A—H8A3	109.5

C3—S1—C1—C2	−0.03 (9)	C4—N2—C5—S2	179.23 (9)
S1—C1—C2—N1	0.23 (13)	C3—N1—C5—N2	3.03 (15)
C3—N1—C2—C1	−0.38 (14)	C2—N1—C5—N2	−178.04 (10)
C5—N1—C2—C1	−179.36 (10)	C3—N1—C5—S2	−177.64 (8)
C4—N3—C3—N1	−1.45 (16)	C2—N1—C5—S2	1.28 (15)
C4—N3—C3—S1	177.43 (9)	C5—N2—C4—N3	−1.78 (19)
C2—N1—C3—N3	179.37 (10)	C5—N2—C4—C6	169.6 (2)
C5—N1—C3—N3	−1.58 (16)	C3—N3—C4—N2	3.24 (19)
C2—N1—C3—S1	0.35 (11)	C3—N3—C4—C6	−167.7 (2)
C5—N1—C3—S1	179.41 (7)	N2—C4—C6—C7	129.4 (3)
C1—S1—C3—N3	−179.19 (10)	N3—C4—C6—C7	−58.6 (4)
C1—S1—C3—N1	−0.19 (8)	C4—C6—C7—C8	−62.5 (5)
C4—N2—C5—N1	−1.48 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N2^{i}	0.95	2.38	3.3261 (16)	171

Symmetry code: (i) −*x*, *y*+1/2, −*z*+1/2.