Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(2,4,6-Trimethylphenyl)-1,3-thiazol-2-amine

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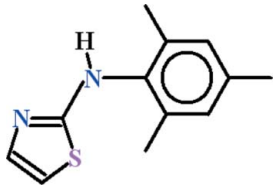
Received 9 July 2012; accepted 10 July 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.116; data-to-parameter ratio = 19.4.

In the title compound, $C_{12}H_{14}N_2S$, the dihedral angle between the 1,3,5-trimethylbenzene and 1,3-thiazol-2-amine groups is 73.15 (4)°. In the crystal, inversion dimers linked by pairs of N—H···N hydrogen bonds generate $R_2^2(8)$ loops.

Related literature

For background to the biological activities of thiazoles, see: Wilson *et al.* (2001). For a related crystal structure, see: Caranoni & Capella (1982).



Experimental

Crystal data

$C_{12}H_{14}N_2S$
M_r = 218.31
Monoclinic, $P2_1/c$
a = 14.2766 (6) Å
b = 7.0676 (2) Å
c = 13.8598 (6) Å
β = 118.736 (2)°
V = 1226.24 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 296 K
0.32 × 0.22 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.929, T_{max} = 0.959
10086 measured reflections
2717 independent reflections
2196 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.116
S = 1.05
2717 reflections
140 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{i}	0.86	2.16	2.944 (2)	151

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the provision of funds for the purchase of the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan. The authors also acknowledge the technical support provided by Syed Muhammad Hussain Rizvi of Bana International, Karachi, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6896).

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supporting information

Acta Cryst. (2012). E**68**, o2441 [https://doi.org/10.1107/S1600536812031315]

N-(2,4,6-Trimethylphenyl)-1,3-thiazol-2-amine

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S1. Comment

Thiazole and its derivatives exhibit a large number of biological properties, for example antifungal and antibacterial (Wilson *et al.*, 2001) activities. As part of our studies in this area, the title compound (I, Fig. 1) has been synthesized and its crystal structure is now reported.

The crystal structures of 1,3-thiazol-2-amine (Caranoni & Capella, 1982) has been published which is related to (I), (Fig. 1).

In (I), the 1,3,5-trimethylbenzene moiety A (C1–C9) and 1,3-thiazol-2-amine group B (N1/C10/S1/C11/C12/N2) are planar with r.m.s. deviation of 0.0345 Å and 0.0031 Å, respectively. The dihedral angle between A/B is 73.15 (4)°. The molecules are linked into dimers due to H-bondings of N—H···N type with $R_2^2(8)$ (Table 1, Fig. 2) ring motif.

S2. Experimental

A mixture of *N*-mesitylthiourea (1 equiv, 1.00 g, 4.58 mmol), 2-chloro-1,1-dimethoxyethane (1.5 equiv, 1.04 g, 6.8 mmol) and few drops of concentrated HCl were dissolved in water and methanol mixture (1:1) (100 ml). The reaction mixture was refluxed for 6 h. The reaction mixture was diluted with water (100 ml) and basified to pH 8 with aqeous NaOH. The resulting precipitate was filtered, washed with cold water and recrystallized from chloroform and hexane (3:1) solution as yellow prisms.

S3. Refinement

The H-atoms were positioned geometrically (C—H = 0.93–0.96 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = xU_{eq}(C, N), where x = 1.5 for methyl groups and x = 1.2 for other H atoms.

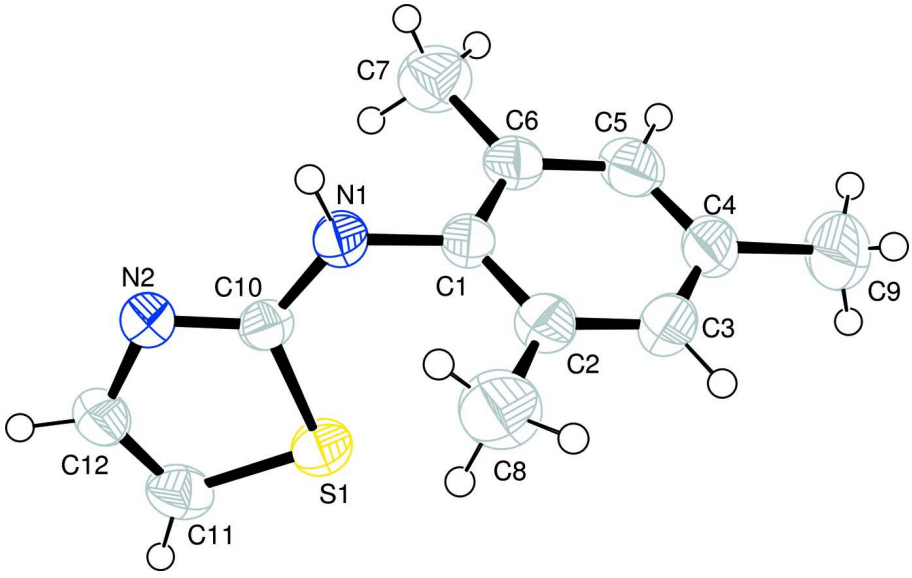

Figure 1

View of the title compound with displacement ellipsoids drawn at the 50% probability level.

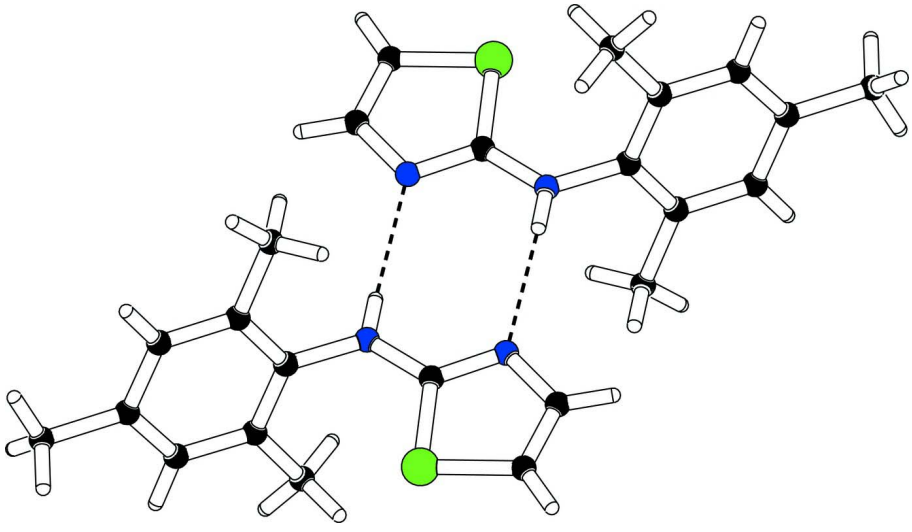

Figure 2

The partial packing (*PLATON*; Spek, 2009) which shows that molecules form dimers with $R_2^2(8)$ loops.

N-(2,4,6-Trimethylphenyl)-1,3-thiazol-2-amine

Crystal data

$C_{12}H_{14}N_2S$
$M_r = 218.31$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.2766\ (6)$ Å
$b = 7.0676\ (2)$ Å
$c = 13.8598\ (6)$ Å
$\beta = 118.736\ (2)°$
$V = 1226.24\ (9)$ Å^3
$Z = 4$
$F(000) = 464$
$D_x = 1.183$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2196 reflections
$\theta = 1.6–27.3°$
$\mu = 0.23$ mm^{-1}

T = 296 K
Prism, yellow

0.32 × 0.22 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.80 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.929, T_{max} = 0.959

10086 measured reflections
2717 independent reflections
2196 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.3°, θ_{min} = 1.6°
h = −18→18
k = −8→9
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.116
S = 1.05
2717 reflections
140 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0574P)^2 + 0.3377P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.049 (4)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > \sigma(F^2)$ 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}
S1	0.28549 (3)	0.60626 (7)	0.20694 (3)	0.0510 (2)
N1	0.37642 (11)	0.6678 (2)	0.42680 (11)	0.0489 (4)
N2	0.46689 (11)	0.4830 (2)	0.35713 (11)	0.0457 (4)
C1	0.28129 (12)	0.7598 (2)	0.41025 (12)	0.0417 (5)
C2	0.25718 (15)	0.9401 (3)	0.36248 (14)	0.0503 (5)
C3	0.16150 (17)	1.0218 (3)	0.34372 (15)	0.0619 (7)
C4	0.09327 (16)	0.9380 (3)	0.37534 (15)	0.0640 (7)
C5	0.12224 (14)	0.7638 (3)	0.42681 (14)	0.0579 (6)
C6	0.21467 (13)	0.6720 (2)	0.44421 (12)	0.0464 (5)
C7	0.24324 (19)	0.4809 (3)	0.49949 (19)	0.0689 (8)
C8	0.3330 (2)	1.0470 (3)	0.3358 (2)	0.0774 (9)
C9	−0.0095 (2)	1.0332 (5)	0.3547 (2)	0.1073 (13)
C10	0.38520 (12)	0.5850 (2)	0.34340 (12)	0.0385 (4)

C11	0.36100 (15)	0.4680 (3)	0.16835 (14)	0.0522 (6)
C12	0.45154 (15)	0.4168 (3)	0.25688 (14)	0.0499 (6)
H1	0.43021	0.66451	0.49200	0.0586*
H3	0.14255	1.13832	0.30825	0.0742*
H5	0.07821	0.70656	0.45048	0.0694*
H7A	0.18460	0.43399	0.50812	0.1034*
H7B	0.30533	0.49271	0.57044	0.1034*
H7C	0.25797	0.39442	0.45505	0.1034*
H8A	0.31727	1.17980	0.33141	0.1162*
H8B	0.32495	1.00412	0.26651	0.1162*
H8C	0.40502	1.02536	0.39246	0.1162*
H9A	−0.05817	1.03567	0.27711	0.1608*
H9B	0.00533	1.16026	0.38250	0.1608*
H9C	−0.04105	0.96399	0.39150	0.1608*
H11	0.34159	0.43378	0.09636	0.0626*
H12	0.50176	0.34047	0.25128	0.0599*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0449 (3)	0.0634 (3)	0.0357 (2)	0.0060 (2)	0.0122 (2)	0.0011 (2)
N1	0.0442 (7)	0.0644 (9)	0.0332 (6)	0.0155 (7)	0.0148 (5)	0.0007 (6)
N2	0.0449 (7)	0.0542 (8)	0.0398 (7)	0.0100 (6)	0.0217 (6)	0.0047 (6)
C1	0.0410 (8)	0.0480 (9)	0.0323 (7)	0.0071 (7)	0.0147 (6)	−0.0023 (6)
C2	0.0594 (10)	0.0491 (9)	0.0441 (9)	0.0067 (8)	0.0263 (8)	0.0009 (7)
C3	0.0747 (13)	0.0597 (11)	0.0479 (10)	0.0267 (10)	0.0268 (9)	0.0082 (8)
C4	0.0539 (10)	0.0921 (15)	0.0403 (9)	0.0287 (10)	0.0182 (8)	0.0018 (9)
C5	0.0448 (9)	0.0857 (14)	0.0432 (9)	0.0020 (9)	0.0212 (7)	−0.0026 (9)
C6	0.0481 (9)	0.0532 (9)	0.0347 (7)	0.0004 (7)	0.0174 (7)	−0.0039 (7)
C7	0.0830 (14)	0.0585 (12)	0.0719 (13)	−0.0024 (10)	0.0425 (12)	0.0080 (10)
C8	0.0980 (17)	0.0590 (12)	0.0915 (17)	−0.0005 (12)	0.0585 (15)	0.0086 (11)
C9	0.0779 (16)	0.166 (3)	0.0768 (16)	0.0672 (19)	0.0362 (13)	0.0210 (17)
C10	0.0377 (7)	0.0420 (8)	0.0340 (7)	0.0021 (6)	0.0158 (6)	0.0044 (6)
C11	0.0656 (11)	0.0535 (10)	0.0407 (8)	−0.0042 (8)	0.0282 (8)	−0.0051 (7)
C12	0.0594 (10)	0.0505 (10)	0.0500 (9)	0.0078 (8)	0.0344 (8)	0.0015 (7)

Geometric parameters (Å, º)

S1—C10	1.7428 (15)	C6—C7	1.509 (3)
S1—C11	1.720 (2)	C11—C12	1.335 (3)
N1—C1	1.421 (2)	C3—H3	0.9300
N1—C10	1.354 (2)	C5—H5	0.9300
N2—C10	1.305 (2)	C7—H7A	0.9600
N2—C12	1.380 (2)	C7—H7B	0.9600
N1—H1	0.8600	C7—H7C	0.9600
C1—C6	1.393 (3)	C8—H8A	0.9600
C1—C2	1.401 (2)	C8—H8B	0.9600
C2—C3	1.388 (3)	C8—H8C	0.9600

C2—C8	1.505 (4)	C9—H9A	0.9600
C3—C4	1.379 (3)	C9—H9B	0.9600
C4—C5	1.383 (3)	C9—H9C	0.9600
C4—C9	1.511 (4)	C11—H11	0.9300
C5—C6	1.384 (3)	C12—H12	0.9300

C10—S1—C11	88.94 (8)	C4—C3—H3	119.00
C1—N1—C10	122.23 (14)	C4—C5—H5	119.00
C10—N2—C12	110.02 (15)	C6—C5—H5	119.00
C1—N1—H1	119.00	C6—C7—H7A	109.00
C10—N1—H1	119.00	C6—C7—H7B	109.00
N1—C1—C2	119.41 (17)	C6—C7—H7C	109.00
N1—C1—C6	119.75 (13)	H7A—C7—H7B	109.00
C2—C1—C6	120.82 (17)	H7A—C7—H7C	109.00
C1—C2—C3	117.6 (2)	H7B—C7—H7C	109.00
C3—C2—C8	120.31 (19)	C2—C8—H8A	109.00
C1—C2—C8	122.1 (2)	C2—C8—H8B	109.00
C2—C3—C4	122.9 (2)	C2—C8—H8C	109.00
C3—C4—C9	121.2 (2)	H8A—C8—H8B	109.00
C3—C4—C5	117.7 (2)	H8A—C8—H8C	109.00
C5—C4—C9	121.1 (2)	H8B—C8—H8C	110.00
C4—C5—C6	122.1 (2)	C4—C9—H9A	110.00
C1—C6—C5	118.75 (15)	C4—C9—H9B	110.00
C5—C6—C7	120.70 (19)	C4—C9—H9C	109.00
C1—C6—C7	120.55 (18)	H9A—C9—H9B	110.00
S1—C10—N2	114.35 (12)	H9A—C9—H9C	109.00
S1—C10—N1	121.78 (13)	H9B—C9—H9C	109.00
N1—C10—N2	123.87 (14)	S1—C11—H11	125.00
S1—C11—C12	110.05 (14)	C12—C11—H11	125.00
N2—C12—C11	116.6 (2)	N2—C12—H12	122.00
C2—C3—H3	119.00	C11—C12—H12	122.00

C11—S1—C10—N1	−179.66 (15)	N1—C1—C6—C5	−179.71 (14)
C11—S1—C10—N2	−0.05 (14)	N1—C1—C6—C7	0.6 (2)
C10—S1—C11—C12	0.38 (17)	C2—C1—C6—C5	2.0 (2)
C10—N1—C1—C2	−76.7 (2)	C2—C1—C6—C7	−177.69 (16)
C10—N1—C1—C6	104.96 (18)	C1—C2—C3—C4	3.6 (3)
C1—N1—C10—S1	6.9 (2)	C8—C2—C3—C4	−174.12 (19)
C1—N1—C10—N2	−172.72 (16)	C2—C3—C4—C5	−0.8 (3)
C12—N2—C10—S1	−0.29 (19)	C2—C3—C4—C9	179.1 (2)
C12—N2—C10—N1	179.31 (17)	C3—C4—C5—C6	−1.7 (3)
C10—N2—C12—C11	0.6 (3)	C9—C4—C5—C6	178.44 (18)
N1—C1—C2—C3	177.48 (15)	C4—C5—C6—C1	1.1 (3)
N1—C1—C2—C8	−4.8 (2)	C4—C5—C6—C7	−179.29 (18)
C6—C1—C2—C3	−4.2 (2)	S1—C11—C12—N2	−0.7 (3)
C6—C1—C2—C8	173.51 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{i}	0.86	2.16	2.944 (2)	151

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