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2-(2-Methylphenyl)-N-(1,3-thiazol-2-yl)-acetamide

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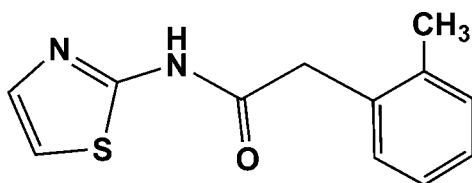
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.040; wR factor = 0.113; data-to-parameter ratio = 15.3.

In the title compound, $\text{C}_{12}\text{H}_{12}\text{N}_2\text{OS}$, the dihedral angle between the benzene and thiazole rings is $83.5(7)^\circ$. The acetamide group is almost coplanar with the thiazole ring, being twisted from it by $4.2(9)^\circ$. In the crystal, pairs of $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds link molecules into inversion dimers, generating $R_2^2[8]$ loops; the dimers are stacked along $[001]$.

Related literature

For the structural similarity of N -substituted 2-arylacetamides to the lateral chain of benzylpenicillin, see: Mijin *et al.* (2008). For our studies of acetamides, see: Nayak *et al.* (2014).



Experimental

Crystal data

 $\text{C}_{12}\text{H}_{12}\text{N}_2\text{OS}$
 $M_r = 232.30$
Monoclinic, $P2_1/c$
 $a = 17.6983(6)$ Å
 $b = 4.94078(13)$ Å
 $c = 14.4603(5)$ Å
 $\beta = 111.236(4)^\circ$ $V = 1178.60(7)$ Å³
 $Z = 4$
Cu $K\alpha$ radiation
 $\mu = 2.28$ mm⁻¹
 $T = 173$ K
 $0.38 \times 0.26 \times 0.14$ mm

Data collection

Agilent Agilent (Eos, Gemini) diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Agilent, 2012)
 $T_{\min} = 0.582$, $T_{\max} = 1.000$ 7059 measured reflections
2250 independent reflections
2065 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.037$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.113$
 $S = 1.07$
2250 reflections147 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.30$ e Å⁻³
 $\Delta\rho_{\min} = -0.28$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{N2}^i$	0.88	2.04	2.9138 (19)	176

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *SUPERFLIP* (Palatinus *et al.*, 2012); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7232).

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supporting information

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2-(2-Methylphenyl)-*N*-(1,3-thiazol-2-yl)acetamide

B. Narayana, Prakash S. Nayak, Balladka K. Sarojini and Jerry P. Jasinski

S1. Comment

N-Substituted 2-arylacetamides are interesting compounds because of their structural similarity to the lateral chain of natural benzylpenicillin (Mijin *et al.*, 2008). As part of our ongoing studies of such systems (Nayak *et al.*, 2014) we report herein the crystal structure of the title compound, (I), C₁₂H₁₂N₂OS.

In (I), the dihedral angle between the mean planes of the phenyl and thiazol rings is 83.5 (7)° (Fig. 1). The acetamide group (N1/O1/C4/C5) is close to coplanar with the mean plane of the thiazol ring twisted by 4.2 (9)°. In the crystal, pairs of N—H···N hydrogen bonds link the molecules into inversion dimers forming R₂²[8] ring motifs and stacked along [001] (Fig. 2).

S2. Experimental

2-Methylphenylacetic acid (0.150 g, 1 mmol), 2-aminothiazole (0.100 g, 1 mmol) and 1-ethyl-3-(3-dimethylamino-propyl)-carbodiimide hydrochloride (1.0 g, 0.01 mol) were dissolved in dichloromethane (20 ml). The mixture was stirred in presence of triethylamine at 273 K for about 3 h. The contents were poured into 100 ml of ice-cold aqueous hydrochloric acid with stirring, which was extracted thrice with dichloromethane. The organic layer was washed with saturated NaHCO₃ solution and brine solution, dried and concentrated under reduced pressure to give the title compound (I). Colourless prisms were grown from methanol solution by slow evaporation (M.P.: 401–403 K).

S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with Atom—H lengths of 0.95 Å (CH), 0.99 Å (CH₂), 0.98 Å (CH₃) or 0.88 Å (NH). Isotropic displacement parameters for these atoms were set to 1.2 (CH, CH₂, NH) or 1.5 (CH₃) times *U*_{eq} of the parent atom. Idealised Me refined as rotating group.

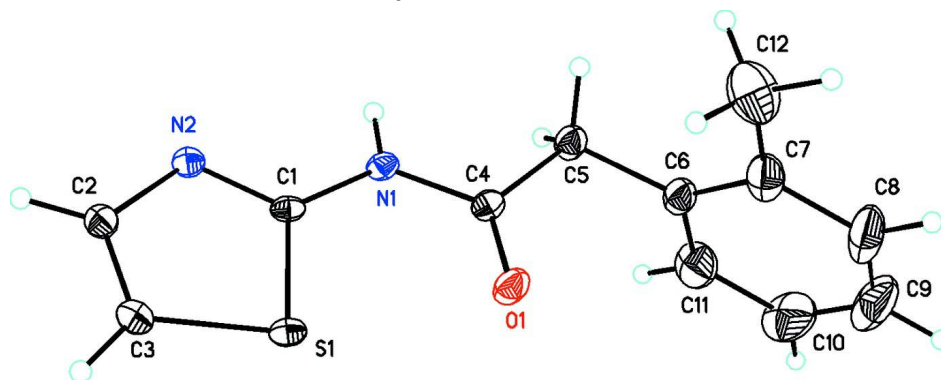
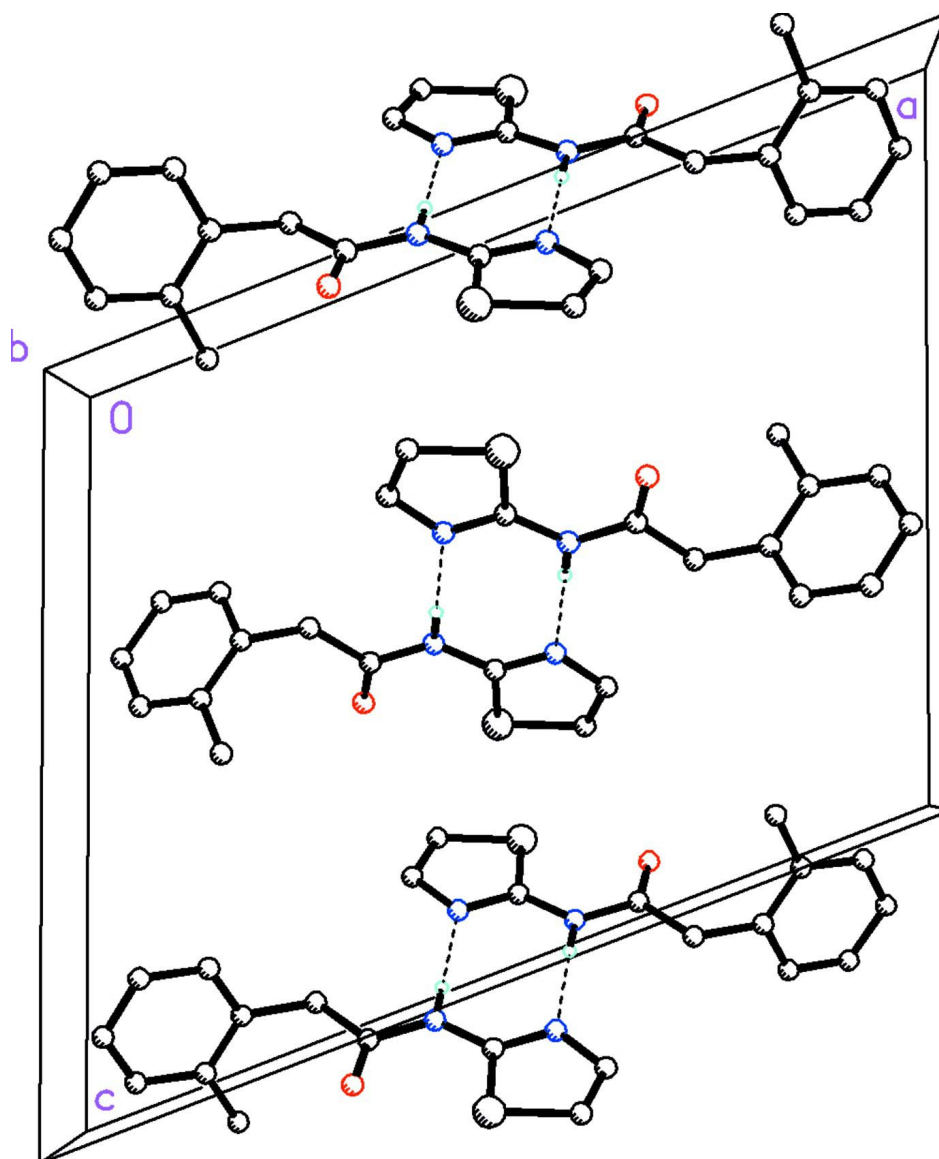


Figure 1

ORTEP drawing of (I), C₁₂H₁₂N₂OS, showing 30% probability displacement ellipsoids.

**Figure 2**

Molecular packing for (I) viewed along the *b* axis. Dashed lines indicate weak N1—H1...N2 hydrogen bonds forming inversion dimers in an $R_2^2[8]$ motif format and stacked along [001]. H atoms not involved in hydrogen bonding have been removed for clarity.

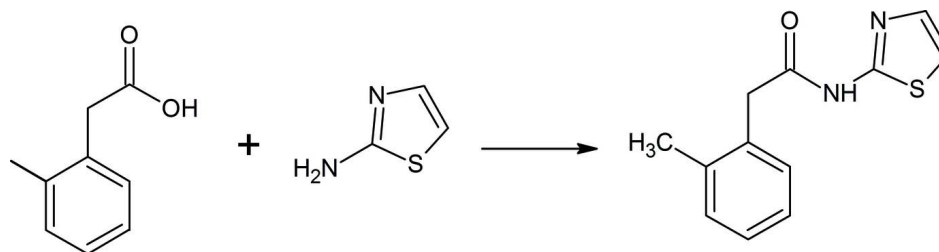


Figure 3

Reaction scheme.

2-(2-Methylphenyl)-N-(1,3-thiazol-2-yl)acetamide*Crystal data*C₁₂H₁₂N₂OS $M_r = 232.30$ Monoclinic, $P2_1/c$ $a = 17.6983$ (6) Å $b = 4.94078$ (13) Å $c = 14.4603$ (5) Å $\beta = 111.236$ (4)° $V = 1178.60$ (7) Å³ $Z = 4$ $F(000) = 488$ $D_x = 1.309$ Mg m⁻³Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 3416 reflections

 $\theta = 3.4$ – 71.5 ° $\mu = 2.28$ mm⁻¹ $T = 173$ K

Prism, colourless

 $0.38 \times 0.26 \times 0.14$ mm*Data collection*Agilent Agilent (Eos, Gemini)
diffractometerRadiation source: Enhance (Cu) X-ray Source
Graphite monochromatorDetector resolution: 16.0416 pixels mm⁻¹ ω scansAbsorption correction: multi-scan
(*CrysAlis RED*; Agilent, 2012) $T_{\min} = 0.582$, $T_{\max} = 1.000$

7059 measured reflections

2250 independent reflections

2065 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.037$ $\theta_{\max} = 71.3$ °, $\theta_{\min} = 5.4$ ° $h = -12 \rightarrow 21$ $k = -5 \rightarrow 6$ $l = -17 \rightarrow 16$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.040$ $wR(F^2) = 0.113$ $S = 1.07$

2250 reflections

147 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0678P)^2 + 0.367P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.30$ e Å⁻³ $\Delta\rho_{\min} = -0.28$ e Å⁻³Extinction correction: *SHELXL2012* (Sheldrick,
2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0013 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.51096 (2)	1.09810 (8)	0.33600 (3)	0.02349 (18)
O1	0.66917 (7)	0.9640 (3)	0.43484 (10)	0.0341 (3)
N1	0.58012 (8)	0.6996 (3)	0.47251 (10)	0.0225 (3)
H1	0.5748	0.5659	0.5099	0.027*

N2	0.43898 (8)	0.7241 (3)	0.39749 (10)	0.0241 (3)
C1	0.51059 (10)	0.8180 (3)	0.40772 (11)	0.0204 (3)
C2	0.38010 (11)	0.8760 (3)	0.32755 (13)	0.0269 (4)
H2	0.3240	0.8362	0.3089	0.032*
C3	0.40679 (11)	1.0842 (3)	0.28727 (13)	0.0263 (4)
H3	0.3730	1.2055	0.2390	0.032*
C4	0.65649 (10)	0.7763 (3)	0.48226 (12)	0.0248 (4)
C5	0.72262 (11)	0.6059 (4)	0.55603 (14)	0.0311 (4)
H5A	0.7121	0.5926	0.6186	0.037*
H5B	0.7205	0.4206	0.5291	0.037*
C6	0.80617 (11)	0.7206 (4)	0.57813 (14)	0.0352 (4)
C7	0.85116 (13)	0.6620 (5)	0.51962 (17)	0.0469 (5)
C8	0.92758 (14)	0.7817 (6)	0.5445 (2)	0.0675 (9)
H8	0.9594	0.7420	0.5055	0.081*
C9	0.95774 (17)	0.9541 (7)	0.6231 (3)	0.0828 (11)
H9	1.0096	1.0343	0.6377	0.099*
C10	0.91323 (19)	1.0119 (7)	0.6813 (3)	0.0811 (10)
H10	0.9339	1.1318	0.7361	0.097*
C11	0.83836 (15)	0.8938 (5)	0.6590 (2)	0.0559 (6)
H11	0.8079	0.9311	0.6998	0.067*
C12	0.81906 (19)	0.4717 (7)	0.4331 (2)	0.0710 (8)
H12A	0.8022	0.3021	0.4550	0.106*
H12B	0.8616	0.4343	0.4064	0.106*
H12C	0.7724	0.5546	0.3814	0.106*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0313 (3)	0.0181 (3)	0.0218 (2)	-0.00228 (14)	0.01054 (18)	0.00177 (13)
O1	0.0295 (7)	0.0335 (7)	0.0382 (7)	-0.0062 (5)	0.0106 (5)	0.0106 (6)
N1	0.0257 (7)	0.0202 (7)	0.0220 (6)	-0.0031 (5)	0.0089 (5)	0.0035 (5)
N2	0.0257 (7)	0.0219 (7)	0.0250 (7)	-0.0004 (5)	0.0096 (5)	0.0022 (5)
C1	0.0294 (8)	0.0159 (7)	0.0183 (7)	-0.0018 (6)	0.0115 (6)	-0.0023 (6)
C2	0.0260 (8)	0.0261 (9)	0.0284 (8)	0.0015 (6)	0.0096 (7)	0.0019 (6)
C3	0.0308 (9)	0.0247 (9)	0.0235 (8)	0.0044 (6)	0.0101 (7)	0.0013 (6)
C4	0.0265 (8)	0.0240 (9)	0.0233 (8)	-0.0034 (6)	0.0085 (7)	-0.0018 (6)
C5	0.0271 (9)	0.0322 (10)	0.0335 (9)	-0.0013 (7)	0.0102 (7)	0.0068 (7)
C6	0.0263 (9)	0.0361 (11)	0.0391 (10)	0.0002 (7)	0.0070 (7)	0.0099 (8)
C7	0.0370 (11)	0.0567 (13)	0.0489 (12)	0.0071 (10)	0.0178 (10)	0.0186 (10)
C8	0.0339 (12)	0.089 (2)	0.0833 (19)	0.0044 (13)	0.0251 (13)	0.0412 (17)
C9	0.0353 (13)	0.090 (2)	0.101 (3)	-0.0176 (14)	-0.0016 (15)	0.037 (2)
C10	0.0568 (17)	0.071 (2)	0.083 (2)	-0.0188 (15)	-0.0131 (15)	-0.0067 (17)
C11	0.0426 (12)	0.0610 (16)	0.0519 (14)	0.0004 (10)	0.0026 (10)	-0.0077 (11)
C12	0.0721 (18)	0.088 (2)	0.0601 (16)	0.0142 (16)	0.0329 (14)	-0.0043 (15)

Geometric parameters (Å, °)

S1—C1	1.7307 (16)	C6—C7	1.386 (3)
S1—C3	1.7202 (18)	C6—C11	1.394 (3)
O1—C4	1.222 (2)	C7—C8	1.399 (3)
N1—H1	0.8800	C7—C12	1.502 (4)
N1—C1	1.378 (2)	C8—H8	0.9500
N1—C4	1.361 (2)	C8—C9	1.365 (5)
N2—C1	1.307 (2)	C9—H9	0.9500
N2—C2	1.382 (2)	C9—C10	1.375 (5)
C2—H2	0.9500	C10—H10	0.9500
C2—C3	1.349 (2)	C10—C11	1.375 (4)
C3—H3	0.9500	C11—H11	0.9500
C4—C5	1.521 (2)	C12—H12A	0.9800
C5—H5A	0.9900	C12—H12B	0.9800
C5—H5B	0.9900	C12—H12C	0.9800
C5—C6	1.506 (2)		
C3—S1—C1	88.70 (8)	C7—C6—C11	119.3 (2)
C1—N1—H1	117.9	C11—C6—C5	118.73 (19)
C4—N1—H1	117.9	C6—C7—C8	118.1 (3)
C4—N1—C1	124.11 (14)	C6—C7—C12	120.8 (2)
C1—N2—C2	109.46 (14)	C8—C7—C12	121.2 (2)
N1—C1—S1	123.41 (12)	C7—C8—H8	119.1
N2—C1—S1	115.48 (12)	C9—C8—C7	121.8 (3)
N2—C1—N1	121.11 (14)	C9—C8—H8	119.1
N2—C2—H2	121.9	C8—C9—H9	120.0
C3—C2—N2	116.18 (16)	C8—C9—C10	120.1 (3)
C3—C2—H2	121.9	C10—C9—H9	120.0
S1—C3—H3	124.9	C9—C10—H10	120.5
C2—C3—S1	110.15 (13)	C9—C10—C11	119.1 (3)
C2—C3—H3	124.9	C11—C10—H10	120.5
O1—C4—N1	122.06 (15)	C6—C11—H11	119.2
O1—C4—C5	124.26 (15)	C10—C11—C6	121.5 (3)
N1—C4—C5	113.67 (14)	C10—C11—H11	119.2
C4—C5—H5A	109.0	C7—C12—H12A	109.5
C4—C5—H5B	109.0	C7—C12—H12B	109.5
H5A—C5—H5B	107.8	C7—C12—H12C	109.5
C6—C5—C4	112.79 (14)	H12A—C12—H12B	109.5
C6—C5—H5A	109.0	H12A—C12—H12C	109.5
C6—C5—H5B	109.0	H12B—C12—H12C	109.5
C7—C6—C5	121.9 (2)		
O1—C4—C5—C6	9.8 (3)	C4—C5—C6—C7	-86.3 (2)
N1—C4—C5—C6	-170.71 (15)	C4—C5—C6—C11	92.8 (2)
N2—C2—C3—S1	0.6 (2)	C5—C6—C7—C8	178.75 (19)
C1—S1—C3—C2	0.12 (13)	C5—C6—C7—C12	-2.2 (3)
C1—N1—C4—O1	1.8 (3)	C5—C6—C11—C10	-177.9 (2)

C1—N1—C4—C5	-177.74 (14)	C6—C7—C8—C9	-0.7 (4)
C1—N2—C2—C3	-1.3 (2)	C7—C6—C11—C10	1.1 (4)
C2—N2—C1—S1	1.36 (17)	C7—C8—C9—C10	0.8 (5)
C2—N2—C1—N1	-179.21 (14)	C8—C9—C10—C11	0.0 (5)
C3—S1—C1—N1	179.70 (14)	C9—C10—C11—C6	-1.0 (5)
C3—S1—C1—N2	-0.89 (13)	C11—C6—C7—C8	-0.3 (3)
C4—N1—C1—S1	-4.9 (2)	C11—C6—C7—C12	178.7 (2)
C4—N1—C1—N2	175.74 (14)	C12—C7—C8—C9	-179.7 (3)

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
N1—H1...N2 ⁱ	0.88	2.04	2.9138 (19)	176

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