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N-(1,3-Thiazol-2-yl)benzamide

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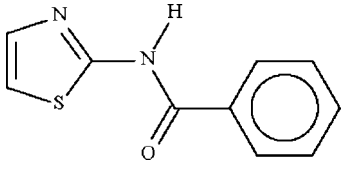
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; R factor = 0.029; wR factor = 0.087; data-to-parameter ratio = 16.1.

The title compound, $C_{10}H_8N_2OS$, features a nonplanar molecule [dihedral angle between the two aromatic rings = 43.6 (1)°]. Two molecules are linked by N—H···N hydrogen bonds about a centre of inversion, giving rise to a hydrogen-bonded dimer.

Related literature

The synthesis uses microwave radiation, which compares with benzoylation by reacting benzoyl cyanide in an ionic liquid: see: Kumar *et al.* (2007); Prasad *et al.* (2005).



Experimental

Crystal data

$C_{10}H_8N_2OS$
M_r = 204.24
Monoclinic, $P2_1/c$
a = 12.0142 (2) Å
b = 5.0581 (1) Å
c = 15.4090 (3) Å
β = 99.093 (1)°
V = 924.62 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 123 K
0.35 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.898, T_{max} = 0.955
6130 measured reflections
2104 independent reflections
1900 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.087
S = 1.07
2104 reflections
131 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 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
N2—H2···N1^{i}	0.88 (2)	2.04 (2)	2.922 (2)	173 (2)

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; 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, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2897).

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supplementary materials

Acta Cryst. (2009). E**65**, o817 [**doi:10.1107/S1600536809009374**]

N-(1,3-Thiazol-2-yl)benzamide

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Comment

(type here to add)

Experimental

2-Aminothiazole (1 g, 10 mmol) and benzoyl cyanide (1.31 g, 10 mmol) were stirred together without any solvent for 3 h at 323 K. The oily product was purified by recrystalization from ethanol (yield 1.97 g, 90%); m.p. 383 K.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.95 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U(C).

The amino H-atom was located in a difference Fouier map, and was freely refined.

Figures

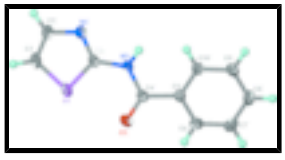

Fig. 1. Anisotropic displacement ellisoid plot (Barbour, 2001) of $C_{10}H_8N_2OS$; probability levels are set at 70% and H-atoms are drawn as spheres of arbitrary radius.

N-(1,3-Thiazol-2-yl)benzamide

Crystal data

$C_{10}H_8N_2OS$	F_{000} = 424
M_r = 204.24	D_x = 1.467 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3661 reflections
a = 12.0142 (2) Å	θ = 2.7–28.3°
b = 5.0581 (1) Å	μ = 0.31 mm^{-1}
c = 15.4090 (3) Å	T = 123 K
β = 99.093 (1)°	Prism, colorless
V = 924.62 (3) Å^3	0.35 × 0.20 × 0.15 mm
Z = 4	

Data collection

Bruker SMART APEX diffractometer	2104 independent reflections
Radiation source: fine-focus sealed tube	1900 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.016$
$T = 123$ K	$\theta_{max} = 27.5^{o}$
ω scans	$\theta_{min} = 1.7^{o}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -15\rightarrow15$
$T_{min} = 0.898$, $T_{max} = 0.955$	$k = -6\rightarrow6$
6130 measured reflections	$l = -18\rightarrow20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.029$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.087$	$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.3231P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
2104 reflections	$\Delta\rho_{max} = 0.37$ e Å^{-3}
131 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.31389 (3)	0.14766 (7)	0.64434 (2)	0.02139 (12)
O1	0.17527 (8)	0.5276 (2)	0.56442 (6)	0.0229 (2)
N1	0.49298 (9)	0.2290 (2)	0.57510 (7)	0.0196 (2)
N2	0.34258 (9)	0.4997 (2)	0.51416 (7)	0.0186 (2)
H2	0.3903 (16)	0.574 (4)	0.4833 (13)	0.039 (5)*
C1	0.43025 (12)	−0.0499 (3)	0.67627 (9)	0.0229 (3)
H1	0.4338	−0.1892	0.7180	0.028*
C2	0.51534 (11)	0.0214 (3)	0.63371 (8)	0.0210 (3)
H2A	0.5863	−0.0656	0.6434	0.025*
C3	0.38904 (11)	0.3090 (2)	0.57304 (8)	0.0173 (3)
C4	0.23427 (11)	0.5903 (3)	0.50994 (8)	0.0179 (3)
C5	0.19345 (10)	0.7638 (3)	0.43320 (8)	0.0178 (3)
C6	0.11908 (11)	0.9675 (3)	0.44382 (9)	0.0207 (3)
H6	0.0981	0.9989	0.4998	0.025*
C7	0.07532 (11)	1.1252 (3)	0.37287 (9)	0.0239 (3)
H7	0.0251	1.2655	0.3804	0.029*

C8	0.10522 (11)	1.0769 (3)	0.29083 (9)	0.0235 (3)
H8	0.0754	1.1848	0.2422	0.028*
C9	0.17835 (11)	0.8722 (3)	0.27946 (9)	0.0221 (3)
H9	0.1978	0.8389	0.2231	0.026*
C10	0.22320 (11)	0.7157 (3)	0.35072 (8)	0.0199 (3)
H10	0.2739	0.5765	0.3432	0.024*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02421 (19)	0.02313 (19)	0.01715 (19)	−0.00215 (12)	0.00419 (13)	0.00464 (12)
O1	0.0245 (5)	0.0273 (5)	0.0181 (5)	0.0007 (4)	0.0071 (4)	0.0020 (4)
N1	0.0231 (5)	0.0187 (5)	0.0170 (5)	0.0014 (4)	0.0027 (4)	0.0016 (4)
N2	0.0201 (5)	0.0202 (5)	0.0160 (5)	0.0008 (4)	0.0049 (4)	0.0042 (4)
C1	0.0300 (7)	0.0190 (6)	0.0181 (6)	−0.0018 (5)	−0.0012 (5)	0.0027 (5)
C2	0.0260 (6)	0.0174 (6)	0.0182 (6)	0.0013 (5)	−0.0010 (5)	0.0002 (5)
C3	0.0223 (6)	0.0170 (6)	0.0125 (6)	−0.0019 (5)	0.0027 (5)	−0.0008 (4)
C4	0.0210 (6)	0.0184 (6)	0.0143 (6)	−0.0004 (5)	0.0028 (5)	−0.0018 (5)
C5	0.0180 (6)	0.0189 (6)	0.0161 (6)	−0.0021 (5)	0.0015 (5)	0.0008 (5)
C6	0.0181 (6)	0.0242 (6)	0.0201 (6)	−0.0001 (5)	0.0038 (5)	−0.0028 (5)
C7	0.0206 (6)	0.0209 (6)	0.0291 (7)	0.0022 (5)	0.0007 (5)	−0.0006 (5)
C8	0.0213 (6)	0.0241 (6)	0.0231 (7)	−0.0013 (5)	−0.0022 (5)	0.0061 (5)
C9	0.0221 (6)	0.0277 (7)	0.0163 (6)	−0.0026 (5)	0.0028 (5)	0.0017 (5)
C10	0.0200 (6)	0.0217 (6)	0.0180 (6)	0.0015 (5)	0.0032 (5)	0.0001 (5)

Geometric parameters (Å, °)

S1—C1	1.7255 (14)	C5—C6	1.3903 (18)
S1—C3	1.7327 (13)	C5—C10	1.3949 (18)
O1—C4	1.2231 (16)	C6—C7	1.3877 (19)
N1—C3	1.3084 (17)	C6—H6	0.9500
N1—C2	1.3834 (16)	C7—C8	1.389 (2)
N2—C4	1.3714 (17)	C7—H7	0.9500
N2—C3	1.3801 (16)	C8—C9	1.387 (2)
N2—H2	0.88 (2)	C8—H8	0.9500
C1—C2	1.348 (2)	C9—C10	1.3913 (18)
C1—H1	0.9500	C9—H9	0.9500
C2—H2A	0.9500	C10—H10	0.9500
C4—C5	1.4919 (17)		
C1—S1—C3	88.49 (6)	C6—C5—C4	118.65 (11)
C3—N1—C2	109.69 (11)	C10—C5—C4	121.33 (12)
C4—N2—C3	123.16 (11)	C7—C6—C5	120.24 (12)
C4—N2—H2	121.6 (13)	C7—C6—H6	119.9
C3—N2—H2	114.8 (13)	C5—C6—H6	119.9
C2—C1—S1	110.43 (10)	C6—C7—C8	119.71 (13)
C2—C1—H1	124.8	C6—C7—H7	120.1
S1—C1—H1	124.8	C8—C7—H7	120.1
C1—C2—N1	115.88 (12)	C7—C8—C9	120.40 (12)

C1—C2—H2A	122.1	C7—C8—H8	119.8
N1—C2—H2A	122.1	C9—C8—H8	119.8
N1—C3—N2	121.17 (11)	C8—C9—C10	119.95 (13)
N1—C3—S1	115.46 (10)	C8—C9—H9	120.0
N2—C3—S1	123.29 (10)	C10—C9—H9	120.0
O1—C4—N2	121.95 (12)	C5—C10—C9	119.78 (12)
O1—C4—C5	122.90 (12)	C5—C10—H10	120.1
N2—C4—C5	115.14 (11)	C9—C10—H10	120.1
C6—C5—C10	119.91 (12)		
C3—S1—C1—C2	1.28 (10)	N2—C4—C5—C6	−146.32 (12)
S1—C1—C2—N1	−0.31 (15)	O1—C4—C5—C10	−141.00 (14)
C3—N1—C2—C1	−1.25 (16)	N2—C4—C5—C10	37.46 (17)
C2—N1—C3—N2	−174.45 (11)	C10—C5—C6—C7	−0.75 (19)
C2—N1—C3—S1	2.29 (14)	C4—C5—C6—C7	−177.03 (11)
C4—N2—C3—N1	−179.70 (12)	C5—C6—C7—C8	0.7 (2)
C4—N2—C3—S1	3.83 (17)	C6—C7—C8—C9	0.1 (2)
C1—S1—C3—N1	−2.12 (10)	C7—C8—C9—C10	−0.7 (2)
C1—S1—C3—N2	174.53 (11)	C6—C5—C10—C9	0.09 (19)
C3—N2—C4—O1	7.78 (19)	C4—C5—C10—C9	176.27 (12)
C3—N2—C4—C5	−170.70 (11)	C8—C9—C10—C5	0.6 (2)
O1—C4—C5—C6	35.22 (18)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N1^{i}	0.88 (2)	2.04 (2)	2.922 (2)	173 (2)

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

Fig. 1