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Methyl 2-[*N*-(thiazol-2-yl)carbamoyl]-benzoate

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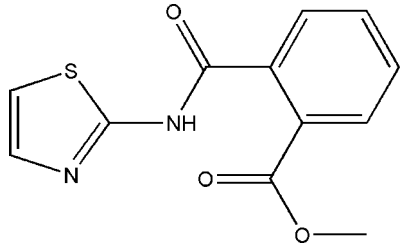
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.113; data-to-parameter ratio = 15.5.

In the title molecule, $C_{12}H_{10}N_2O_3S$, the dihedral angle between the thiazole ring and benzene ring is 87.5 (2)°. In the crystal structure, intermolecular N—H···N hydrogen bonds form centrosymmetric dimers. There is an intramolecular C—H···O interaction.

Related literature

The bond lengths and angles of the title compound agree with those of *N*-(2-bromothiazol-5-ylmethyl)phthalimide (Li *et al.*, 2006).



Experimental

Crystal data

$C_{12}H_{10}N_2O_3S$
M_r = 262.28
Orthorhombic, *Pbca*
a = 14.921 (7) Å
b = 8.885 (5) Å
c = 18.954 (10) Å
V = 2513 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 294 (2) K
0.24 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.941, T_{max} = 0.950
13481 measured reflections
2608 independent reflections
1727 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.113
S = 1.02
2608 reflections
168 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1^{i}	0.86 (2)	2.06 (2)	2.913 (3)	175
C9—H9···O3	0.93	2.40	2.725 (3)	100

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2365).

References

Bruker (1997). *SADABS* (Version 2.01), *SMART* (Version 5.044), *SAINT* (Version 5.01) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Li, J.-T., Wang, J.-K. & Zhou, L.-N. (2006). *Acta Cryst.* E**62**, o2327–o2328.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E**63**, o2819 [**doi:10.1107/S1600536807021241**]

Methyl 2-[*N*-(thiazol-2-yl)carbamoyl]benzoate

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Comment

Thiazole and its derivatives are widely used in the fields of biology and for the synthesis of antibiotic and antipyrotic materials. In this paper, the structure of the title compound, (I), is reported. The molecular structure of (I) is illustrated in Fig. 1. The bond lengths and angles of the title compound agree with those common to *N*-(2-Bromothiazol-5-ylmethyl)phthalimide (Li *et al.*, 2006). The dihedral angle between the thiazole ring and benzene ring is 87.5 (2) °. In the crystal structure, centrosymmetric dimers are formed via intermolecular N—H···N hydrogen bonds (Fig. 2 and Table 1) and a weak intramolecular C—H···O hydrogen bond may influence the conformation of the molecule.

Experimental

Isobenzofuran-1,3-dione (0.02 mol) in methanol (15 ml) was refluxed for 0.5 h, and then cooled. Thiazol-2-amine (0.02 mol) was added to the above solution and was refluxed for 4 h. After cooling, filtration and drying, the title compound was obtained. 10 mg of (I) was dissolved in 10 ml acetone, and the solution was kept at room temperature for 10 d. Natural evaporation gave light yellow single crystals of the title compound, suitable for X-ray analysis.

Refinement

The H atoms bonded to C atoms were positioned geometrically (C—H = 0.93-0.96 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5\ U_{eq}$(methyl C). The H atom bonded to N2 was refined isotropically.

Figures

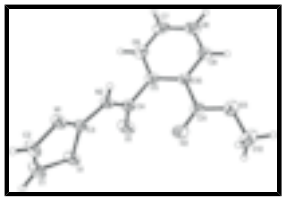

Fig. 1. The molecular structure of (I), drawn with 30% probability ellipsoids.

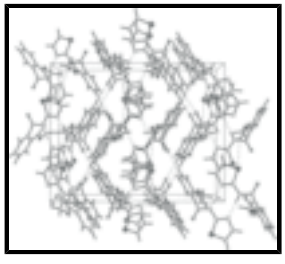

Fig. 2. The crystal packing of (I), viewed along b axis. Hydrogen bonds are indicated by dashed lines.

methyl 2-(thiazol-2-ylcarbamoyl)benzoate

Crystal data

$C_{12}H_{10}N_2O_3S$	F_{000} = 1088
M_r = 262.28	D_x = 1.387 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3562 reflections
a = 14.921 (7) Å	θ = 2.6–25.8º
b = 8.885 (5) Å	μ = 0.26 mm^{-1}
c = 18.954 (10) Å	*T* = 294 (2) K
V = 2513 (2) Å^3	Block, light yellow
Z = 8	0.24 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer	2608 independent reflections
Radiation source: fine-focus sealed tube	1727 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
T = 294(2) K	θ_{max} = 26.5º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	*h* = −9→18
T_{min} = 0.941, T_{max} = 0.950	*k* = −11→10
13481 measured reflections	*l* = −23→23

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.5869P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.040	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.113	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
S = 1.03	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
2608 reflections	Extinction correction: none
168 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.73851 (3)	0.02588 (8)	0.42504 (3)	0.0567 (2)
N2	0.55727 (10)	0.07951 (18)	0.41824 (8)	0.0384 (4)
O1	0.63380 (10)	0.1711 (2)	0.32477 (8)	0.0662 (5)
O2	0.54989 (12)	0.43035 (19)	0.41001 (10)	0.0751 (5)
O3	0.44802 (11)	0.59151 (18)	0.37036 (9)	0.0646 (5)
N1	0.61790 (10)	−0.0419 (2)	0.51622 (9)	0.0471 (4)
C1	0.77031 (14)	−0.0651 (3)	0.50073 (12)	0.0654 (7)
H1	0.8289	−0.0922	0.5116	0.078*
C2	0.69962 (14)	−0.0916 (3)	0.54175 (12)	0.0585 (6)
H2	0.7048	−0.1405	0.5849	0.070*
C3	0.62959 (12)	0.0223 (2)	0.45511 (9)	0.0364 (4)
C4	0.56328 (12)	0.1532 (2)	0.35544 (10)	0.0399 (5)
C5	0.47413 (12)	0.1974 (2)	0.32457 (9)	0.0380 (4)
C6	0.42858 (14)	0.0902 (2)	0.28470 (10)	0.0485 (5)
H6	0.4521	−0.0063	0.2801	0.058*
C7	0.34829 (16)	0.1262 (3)	0.25173 (11)	0.0598 (6)
H7	0.3182	0.0538	0.2254	0.072*
C8	0.31331 (16)	0.2682 (3)	0.25796 (13)	0.0659 (7)
H8	0.2598	0.2922	0.2355	0.079*
C9	0.35732 (15)	0.3755 (3)	0.29740 (12)	0.0569 (6)
H9	0.3332	0.4716	0.3014	0.068*
C10	0.43748 (12)	0.3416 (2)	0.33131 (9)	0.0397 (5)
C11	0.48523 (14)	0.4555 (2)	0.37476 (11)	0.0453 (5)
C12	0.4931 (2)	0.7107 (3)	0.40852 (16)	0.0859 (9)
H12A	0.5015	0.6807	0.4567	0.129*
H12B	0.4573	0.8004	0.4069	0.129*
H12C	0.5503	0.7299	0.3872	0.129*
H2A	0.5057 (14)	0.075 (2)	0.4383 (10)	0.042 (6)*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

S1	0.0282 (3)	0.0935 (5)	0.0485 (3)	0.0046 (3)	0.0109 (2)	0.0111 (3)
N2	0.0248 (8)	0.0530 (10)	0.0373 (9)	−0.0002 (7)	0.0078 (7)	0.0077 (7)
O1	0.0361 (8)	0.1083 (13)	0.0543 (9)	−0.0039 (8)	0.0139 (7)	0.0255 (9)
O2	0.0716 (12)	0.0633 (11)	0.0904 (13)	−0.0096 (9)	−0.0457 (10)	−0.0053 (9)
O3	0.0687 (11)	0.0502 (10)	0.0749 (11)	−0.0021 (8)	−0.0053 (8)	−0.0082 (8)
N1	0.0304 (8)	0.0699 (12)	0.0412 (9)	0.0042 (8)	0.0065 (7)	0.0133 (8)
C1	0.0334 (12)	0.106 (2)	0.0564 (14)	0.0159 (12)	0.0024 (10)	0.0109 (13)
C2	0.0372 (12)	0.0905 (18)	0.0479 (12)	0.0139 (12)	0.0010 (10)	0.0168 (12)
C3	0.0275 (9)	0.0450 (11)	0.0366 (10)	0.0005 (8)	0.0050 (7)	−0.0006 (9)
C4	0.0342 (10)	0.0509 (12)	0.0347 (10)	−0.0026 (9)	0.0054 (8)	0.0018 (9)
C5	0.0349 (10)	0.0505 (12)	0.0286 (9)	−0.0086 (9)	0.0035 (7)	0.0050 (9)
C6	0.0549 (13)	0.0525 (13)	0.0380 (11)	−0.0120 (10)	0.0037 (9)	−0.0016 (9)
C7	0.0609 (14)	0.0755 (17)	0.0430 (12)	−0.0280 (13)	−0.0145 (10)	−0.0002 (12)
C8	0.0515 (14)	0.0804 (18)	0.0659 (15)	−0.0114 (13)	−0.0307 (12)	0.0148 (13)
C9	0.0478 (13)	0.0577 (14)	0.0651 (14)	−0.0021 (11)	−0.0173 (10)	0.0106 (12)
C10	0.0354 (10)	0.0463 (12)	0.0374 (10)	−0.0095 (9)	−0.0060 (8)	0.0060 (8)
C11	0.0450 (12)	0.0468 (13)	0.0441 (11)	−0.0098 (10)	−0.0016 (9)	0.0045 (9)
C12	0.104 (2)	0.0569 (17)	0.097 (2)	−0.0212 (15)	0.0113 (18)	−0.0230 (15)

Geometric parameters (Å, °)

S1—C1	1.714 (2)	C5—C6	1.393 (3)
S1—C3	1.7224 (19)	C5—C10	1.399 (3)
N2—C4	1.362 (2)	C6—C7	1.389 (3)
N2—C3	1.382 (2)	C6—H6	0.9300
N2—H2A	0.86 (2)	C7—C8	1.370 (3)
O1—C4	1.213 (2)	C7—H7	0.9300
O2—C11	1.194 (2)	C8—C9	1.378 (3)
O3—C11	1.333 (3)	C8—H8	0.9300
O3—C12	1.448 (3)	C9—C10	1.391 (3)
N1—C3	1.303 (2)	C9—H9	0.9300
N1—C2	1.384 (3)	C10—C11	1.487 (3)
C1—C2	1.331 (3)	C12—H12A	0.9600
C1—H1	0.9300	C12—H12B	0.9600
C2—H2	0.9300	C12—H12C	0.9600
C4—C5	1.505 (3)		
?···?	?		
C1—S1—C3	88.60 (10)	C5—C6—H6	119.8
C4—N2—C3	124.56 (16)	C8—C7—C6	120.1 (2)
C4—N2—H2A	117.9 (13)	C8—C7—H7	119.9
C3—N2—H2A	117.3 (13)	C6—C7—H7	119.9
C11—O3—C12	116.0 (2)	C7—C8—C9	120.1 (2)
C3—N1—C2	109.42 (16)	C7—C8—H8	119.9
C2—C1—S1	110.66 (17)	C9—C8—H8	119.9
C2—C1—H1	124.7	C8—C9—C10	120.7 (2)
S1—C1—H1	124.7	C8—C9—H9	119.6
C1—C2—N1	115.9 (2)	C10—C9—H9	119.6
C1—C2—H2	122.0	C9—C10—C5	119.50 (18)
N1—C2—H2	122.0	C9—C10—C11	121.4 (2)

N1—C3—N2	120.38 (16)	C5—C10—C11	119.11 (17)
N1—C3—S1	115.37 (14)	O2—C11—O3	122.7 (2)
N2—C3—S1	124.23 (14)	O2—C11—C10	124.7 (2)
O1—C4—N2	122.64 (18)	O3—C11—C10	112.52 (18)
O1—C4—C5	123.11 (17)	O3—C12—H12A	109.5
N2—C4—C5	114.02 (15)	O3—C12—H12B	109.5
C6—C5—C10	119.03 (18)	H12A—C12—H12B	109.5
C6—C5—C4	117.61 (18)	O3—C12—H12C	109.5
C10—C5—C4	123.30 (17)	H12A—C12—H12C	109.5
C7—C6—C5	120.5 (2)	H12B—C12—H12C	109.5
C7—C6—H6	119.8		
C3—S1—C1—C2	0.3 (2)	C4—C5—C6—C7	−176.65 (17)
S1—C1—C2—N1	−0.2 (3)	C5—C6—C7—C8	0.3 (3)
C3—N1—C2—C1	0.0 (3)	C6—C7—C8—C9	−0.5 (4)
C2—N1—C3—N2	179.05 (18)	C7—C8—C9—C10	0.0 (4)
C2—N1—C3—S1	0.2 (2)	C8—C9—C10—C5	0.7 (3)
C4—N2—C3—N1	177.45 (19)	C8—C9—C10—C11	−179.2 (2)
C4—N2—C3—S1	−3.8 (3)	C6—C5—C10—C9	−0.9 (3)
C1—S1—C3—N1	−0.29 (18)	C4—C5—C10—C9	176.01 (18)
C1—S1—C3—N2	−179.07 (18)	C6—C5—C10—C11	179.03 (17)
C3—N2—C4—O1	2.5 (3)	C4—C5—C10—C11	−4.1 (3)
C3—N2—C4—C5	177.13 (17)	C12—O3—C11—O2	2.8 (3)
O1—C4—C5—C6	90.0 (2)	C12—O3—C11—C10	−177.14 (19)
N2—C4—C5—C6	−84.6 (2)	C9—C10—C11—O2	173.3 (2)
O1—C4—C5—C10	−87.0 (3)	C5—C10—C11—O2	−6.7 (3)
N2—C4—C5—C10	98.4 (2)	C9—C10—C11—O3	−6.8 (3)
C10—C5—C6—C7	0.4 (3)	C5—C10—C11—O3	173.25 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···N1^{i}	0.86 (2)	2.06 (2)	2.913 (3)	175
C9—H9···O3	0.93	2.40	2.725 (3)	100

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

Fig. 1

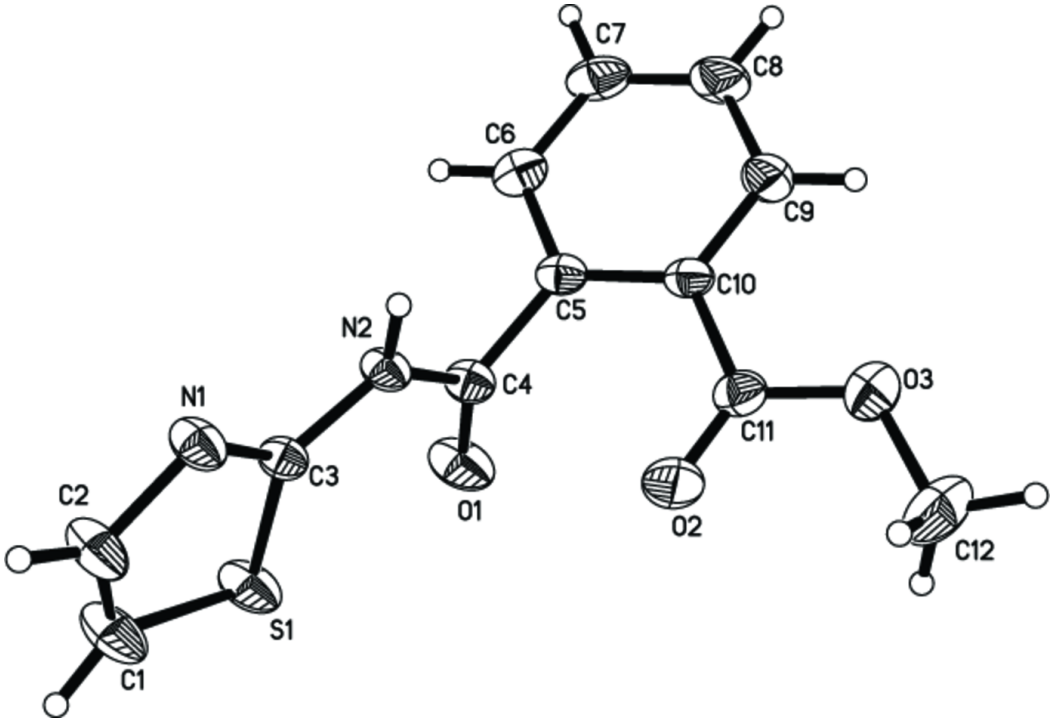

Fig. 2