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Methyl 2-(*p*-toluenesulfonamido)-benzoate

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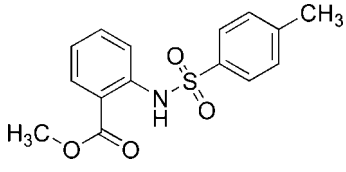
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.102; data-to-parameter ratio = 13.8.

The title compound, $C_{15}H_{15}NO_4S$, was prepared by simple condensation of methyl 2-aminobenzoate and 4-methylbenzenesulfonyl chloride. The dihedral angle between the benzene rings is 84.36 (6)°. The molecular structure is stabilized by an intramolecular N—H···O hydrogen-bonding interaction involving the carbonyl group as acceptor, generating an S(6) graph-set motif.

Related literature

For background information on sulfonamide derivatives and their properties, see: Sheppard *et al.* (2006). For similar structures, see: Schultz *et al.* (2001); Krishnaiah *et al.* (1995); Arshad, Khan, Shafiq *et al.* (2009); Arshad, Khan, Akkurt *et al.* (2009); Xiong *et al.* (2007).



Experimental

Crystal data

$C_{15}H_{15}NO_4S$
M_r = 305.34
Monoclinic, $P2_1/c$
a = 15.0129 (13) Å
b = 8.3593 (7) Å
c = 11.9664 (11) Å
β = 96.854 (2)°
V = 1491.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 295 K
0.24 × 0.16 × 0.14 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.947, T_{max} = 0.968
7663 measured reflections
2639 independent reflections
2230 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.102
S = 1.04
2639 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.87	1.89	2.640 (2)	143

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: BH2263).

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supporting information

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Methyl 2-(*p*-toluenesulfonamido)benzoate

Guang-You Zhang, Di-Juan Chen, Xiang-Yang Guo, Shu-Hong Wang and Jian-Guo Chang

S1. Comment

Sulfur-containing compounds, such as sulfates, sulfones, thiols, sulfonamides and sulfoxides can exhibit insecticidal, germicidal or antimicrobial activities (Schultz *et al.*, 2001; Krishnaiah *et al.*, 1995; Arshad, Khan, Shafiq *et al.*, 2009; Xiong *et al.*, 2007). Particularly, the sulfonamides are biologically active organic compounds, which have been investigated as inhibitors of methionine aminopeptidase-2 (MetAP2) and intermediates for cancer therapy (Sheppard *et al.*, 2006). In order to obtain detailed information on the molecular conformation, the X-ray study of the title sulfonamide has been carried out, and the results are presented here.

As is shown in Fig. 1, the two benzene rings are approximately orthogonal, the dihedral angle between their planes being 84.36 (6)°. In addition to van der Waals interactions, there is an intramolecular N—H···O hydrogen bond which generates a graph set motif *S*(6) (Arshad, Khan, Akkurt *et al.*, 2009) to stabilize the molecular conformation (Fig. 1 and Table 1).

S2. Experimental

Methyl 2-aminobenzoate (5 mmol) was dissolved in tetrahydrofuran (10 ml) in a round bottom flask (50 ml). The pH of the solution was maintained at 7–8 using Et_3N. 4-Toluene sulfonyl chloride (6 mmol) was suspended to the above solution and refluxed until all the 4-toluene sulfonyl chloride was consumed. After removal of the solvent, water (20 ml) was added to the residue. Then the mixture was extracted with CH_2Cl_2, and the organic layer was dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure. Further purification was carried out by recrystallization in ethanol to give a solid (yield 83.7%). Single crystals suitable for X-ray analysis were obtained by diffusion of *n*-hexane in an ethanol solution.

S3. Refinement

All C-bonded H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 (aromatic) or 0.96 Å (methyl). Amine H atom H1 was found in a difference map, and its position fixed in final cycles. Isotropic displacement parameters for H atoms were calculated as U_{iso}(H) = 1.5U_{eq}(carrier C, N) for methyl H atoms and H1, and U_{iso}(H) = 1.2U_{eq}(carrier C) for others.

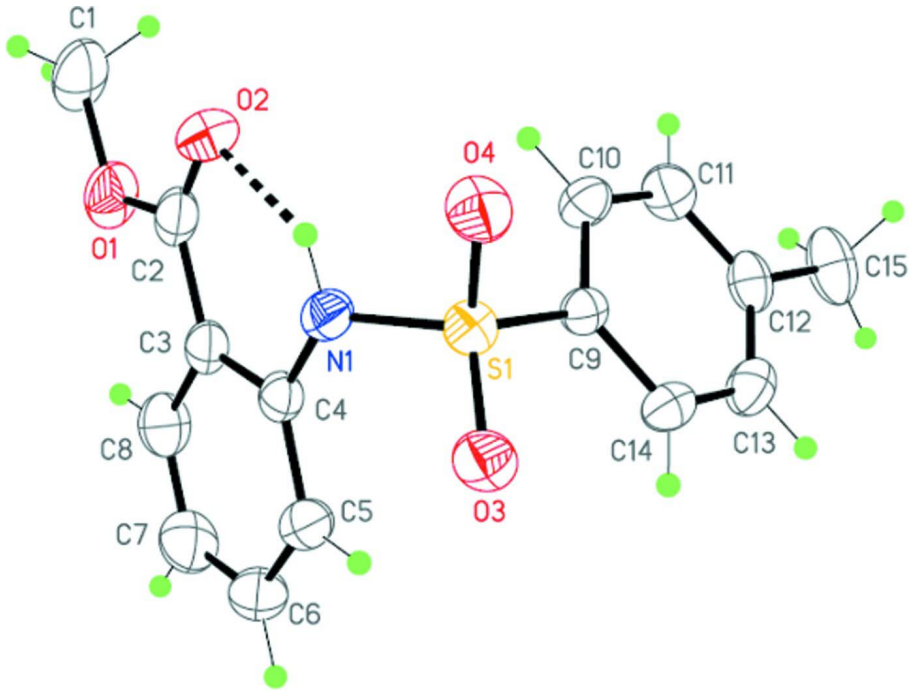

Figure 1

The structure of the title compound with 30% probability ellipsoids. H atoms are shown as spheres of arbitrary radii. The dashed line represents a hydrogen bond.

Methyl 2-(*p*-toluenesulfonamido)benzoate

Crystal data

$C_{15}H_{15}NO_4S$
$M_r = 305.34$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.0129\ (13)$ Å
$b = 8.3593\ (7)$ Å
$c = 11.9664\ (11)$ Å
$\beta = 96.854\ (2)°$
$V = 1491.0\ (2)$ Å^3
$Z = 4$

$F(000) = 640$
$D_x = 1.360$ Mg m^{-3}
Melting point: 380 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3425 reflections
$\theta = 2.3–27.0°$
$\mu = 0.23$ mm^{-1}
$T = 295$ K
Block, colourless
0.24 × 0.16 × 0.14 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.947$, $T_{max} = 0.968$

7663 measured reflections
2639 independent reflections
2230 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.1°$, $\theta_{min} = 2.7°$
$h = -16\rightarrow17$
$k = -9\rightarrow9$
$l = -14\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.102$
$S = 1.04$
2639 reflections
191 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
$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.3683P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.78611 (3)	0.16418 (5)	0.77097 (4)	0.04976 (17)
O1	0.56582 (10)	0.0349 (2)	0.36179 (12)	0.0866 (5)
O2	0.61287 (10)	0.2115 (2)	0.49515 (14)	0.0784 (4)
O3	0.80078 (9)	0.05619 (17)	0.86305 (10)	0.0642 (4)
O4	0.76453 (10)	0.32689 (16)	0.79146 (12)	0.0677 (4)
N1	0.70193 (9)	0.10160 (18)	0.68303 (13)	0.0536 (4)
H1	0.6798	0.1762	0.6367	0.082 (7)*
C1	0.52814 (17)	0.1643 (4)	0.2920 (2)	0.1100 (11)
H1A	0.4763	0.2057	0.3221	0.165*
H1B	0.5111	0.1258	0.2169	0.165*
H1C	0.5720	0.2477	0.2906	0.165*
C2	0.60786 (12)	0.0751 (3)	0.46213 (17)	0.0623 (5)
C3	0.64536 (11)	−0.0668 (2)	0.52490 (15)	0.0524 (4)
C4	0.69256 (10)	−0.0513 (2)	0.63324 (14)	0.0474 (4)
C5	0.72532 (13)	−0.1874 (2)	0.68995 (18)	0.0604 (5)
H5	0.7568	−0.1781	0.7615	0.072*
C6	0.71195 (15)	−0.3359 (2)	0.6419 (2)	0.0748 (6)
H6	0.7343	−0.4261	0.6812	0.090*
C7	0.66594 (16)	−0.3525 (3)	0.5364 (2)	0.0810 (7)
H7	0.6571	−0.4534	0.5042	0.097*
C8	0.63345 (15)	−0.2203 (3)	0.47946 (19)	0.0716 (6)
H8	0.6023	−0.2324	0.4080	0.086*
C9	0.88094 (11)	0.16066 (19)	0.69848 (13)	0.0436 (4)
C10	0.88227 (13)	0.2541 (2)	0.60377 (15)	0.0556 (5)
H10	0.8323	0.3146	0.5766	0.067*
C11	0.95774 (14)	0.2569 (3)	0.55021 (16)	0.0626 (5)
H11	0.9585	0.3201	0.4864	0.075*
C12	1.03322 (12)	0.1678 (2)	0.58876 (16)	0.0581 (5)
C13	1.03009 (13)	0.0749 (2)	0.68292 (17)	0.0623 (5)
H13	1.0800	0.0144	0.7101	0.075*
C14	0.95457 (12)	0.0694 (2)	0.73804 (15)	0.0541 (4)
H14	0.9533	0.0048	0.8011	0.065*
C15	1.11567 (15)	0.1736 (3)	0.5291 (2)	0.0877 (8)
H15A	1.1455	0.2744	0.5438	0.132*

H15B	1.0988	0.1620	0.4495	0.132*
H15C	1.1555	0.0883	0.5557	0.132*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0530 (3)	0.0496 (3)	0.0468 (3)	−0.00029 (19)	0.00665 (19)	−0.00452 (18)
O1	0.0675 (9)	0.1255 (14)	0.0618 (9)	−0.0107 (9)	−0.0128 (7)	0.0207 (9)
O2	0.0743 (10)	0.0717 (10)	0.0861 (11)	0.0118 (8)	−0.0036 (8)	0.0221 (9)
O3	0.0755 (9)	0.0734 (9)	0.0435 (7)	−0.0095 (7)	0.0067 (6)	0.0063 (6)
O4	0.0695 (9)	0.0557 (8)	0.0801 (9)	0.0029 (6)	0.0177 (7)	−0.0180 (7)
N1	0.0498 (8)	0.0470 (8)	0.0620 (9)	0.0048 (7)	−0.0016 (7)	−0.0006 (7)
C1	0.0695 (15)	0.170 (3)	0.0853 (17)	−0.0053 (16)	−0.0123 (13)	0.0621 (19)
C2	0.0391 (9)	0.0881 (16)	0.0591 (12)	−0.0040 (10)	0.0037 (8)	0.0139 (11)
C3	0.0395 (9)	0.0634 (11)	0.0542 (10)	−0.0029 (8)	0.0053 (7)	0.0010 (9)
C4	0.0382 (8)	0.0497 (10)	0.0549 (10)	0.0001 (7)	0.0078 (7)	−0.0011 (8)
C5	0.0592 (11)	0.0540 (11)	0.0657 (12)	0.0030 (9)	−0.0018 (9)	0.0046 (9)
C6	0.0740 (14)	0.0486 (12)	0.1004 (17)	0.0041 (10)	0.0046 (13)	0.0025 (11)
C7	0.0807 (15)	0.0570 (13)	0.1052 (19)	−0.0042 (11)	0.0099 (14)	−0.0210 (13)
C8	0.0667 (13)	0.0823 (15)	0.0642 (13)	−0.0117 (11)	0.0007 (10)	−0.0163 (11)
C9	0.0478 (9)	0.0432 (9)	0.0384 (8)	0.0004 (7)	−0.0004 (7)	−0.0031 (7)
C10	0.0557 (11)	0.0626 (12)	0.0470 (10)	0.0063 (9)	0.0004 (8)	0.0076 (8)
C11	0.0692 (13)	0.0724 (14)	0.0463 (10)	−0.0107 (10)	0.0077 (9)	0.0042 (9)
C12	0.0525 (11)	0.0652 (12)	0.0572 (11)	−0.0128 (9)	0.0091 (9)	−0.0235 (9)
C13	0.0495 (11)	0.0650 (12)	0.0705 (13)	0.0103 (9)	−0.0010 (9)	−0.0100 (10)
C14	0.0588 (11)	0.0532 (11)	0.0484 (10)	0.0087 (8)	−0.0013 (8)	0.0033 (8)
C15	0.0654 (14)	0.109 (2)	0.0933 (17)	−0.0258 (13)	0.0296 (12)	−0.0401 (15)

Geometric parameters (Å, º)

S1—O3	1.4212 (13)	C6—H6	0.9300
S1—O4	1.4262 (14)	C7—C8	1.358 (3)
S1—N1	1.6311 (15)	C7—H7	0.9300
S1—C9	1.7535 (17)	C8—H8	0.9300
O1—C2	1.331 (2)	C9—C10	1.379 (2)
O1—C1	1.440 (3)	C9—C14	1.380 (2)
O2—C2	1.206 (3)	C10—C11	1.367 (3)
N1—C4	1.410 (2)	C10—H10	0.9300
N1—H1	0.8734	C11—C12	1.388 (3)
C1—H1A	0.9600	C11—H11	0.9300
C1—H1B	0.9600	C12—C13	1.374 (3)
C1—H1C	0.9600	C12—C15	1.502 (3)
C2—C3	1.479 (3)	C13—C14	1.379 (3)
C3—C8	1.397 (3)	C13—H13	0.9300
C3—C4	1.407 (2)	C14—H14	0.9300
C4—C5	1.385 (2)	C15—H15A	0.9600
C5—C6	1.373 (3)	C15—H15B	0.9600
C5—H5	0.9300	C15—H15C	0.9600

C6—C7	1.372 (3)		
O3—S1—O4	119.33 (9)	C8—C7—C6	119.4 (2)
O3—S1—N1	109.45 (8)	C8—C7—H7	120.3
O4—S1—N1	104.03 (8)	C6—C7—H7	120.3
O3—S1—C9	108.24 (8)	C7—C8—C3	122.0 (2)
O4—S1—C9	108.40 (8)	C7—C8—H8	119.0
N1—S1—C9	106.73 (8)	C3—C8—H8	119.0
C2—O1—C1	116.4 (2)	C10—C9—C14	120.39 (17)
C4—N1—S1	126.43 (12)	C10—C9—S1	119.30 (13)
C4—N1—H1	111.6	C14—C9—S1	120.27 (13)
S1—N1—H1	112.8	C11—C10—C9	119.29 (17)
O1—C1—H1A	109.5	C11—C10—H10	120.4
O1—C1—H1B	109.5	C9—C10—H10	120.4
H1A—C1—H1B	109.5	C10—C11—C12	121.63 (18)
O1—C1—H1C	109.5	C10—C11—H11	119.2
H1A—C1—H1C	109.5	C12—C11—H11	119.2
H1B—C1—H1C	109.5	C13—C12—C11	117.99 (17)
O2—C2—O1	122.6 (2)	C13—C12—C15	121.3 (2)
O2—C2—C3	125.93 (19)	C11—C12—C15	120.7 (2)
O1—C2—C3	111.5 (2)	C12—C13—C14	121.46 (18)
C8—C3—C4	118.07 (18)	C12—C13—H13	119.3
C8—C3—C2	121.06 (18)	C14—C13—H13	119.3
C4—C3—C2	120.86 (17)	C13—C14—C9	119.23 (17)
C5—C4—C3	119.06 (17)	C13—C14—H14	120.4
C5—C4—N1	121.75 (16)	C9—C14—H14	120.4
C3—C4—N1	119.14 (16)	C12—C15—H15A	109.5
C6—C5—C4	120.82 (19)	C12—C15—H15B	109.5
C6—C5—H5	119.6	H15A—C15—H15B	109.5
C4—C5—H5	119.6	C12—C15—H15C	109.5
C7—C6—C5	120.6 (2)	H15A—C15—H15C	109.5
C7—C6—H6	119.7	H15B—C15—H15C	109.5
C5—C6—H6	119.7		
O3—S1—N1—C4	−53.87 (17)	C6—C7—C8—C3	0.0 (4)
O4—S1—N1—C4	177.55 (15)	C4—C3—C8—C7	−0.1 (3)
C9—S1—N1—C4	63.05 (16)	C2—C3—C8—C7	−178.8 (2)
C1—O1—C2—O2	1.7 (3)	O3—S1—C9—C10	178.84 (13)
C1—O1—C2—C3	−178.72 (17)	O4—S1—C9—C10	−50.38 (16)
O2—C2—C3—C8	178.3 (2)	N1—S1—C9—C10	61.13 (15)
O1—C2—C3—C8	−1.3 (2)	O3—S1—C9—C14	−3.30 (16)
O2—C2—C3—C4	−0.4 (3)	O4—S1—C9—C14	127.47 (15)
O1—C2—C3—C4	−179.97 (15)	N1—S1—C9—C14	−121.02 (14)
C8—C3—C4—C5	0.2 (3)	C14—C9—C10—C11	−0.8 (3)
C2—C3—C4—C5	178.93 (16)	S1—C9—C10—C11	177.06 (14)
C8—C3—C4—N1	−177.13 (16)	C9—C10—C11—C12	0.1 (3)
C2—C3—C4—N1	1.6 (2)	C10—C11—C12—C13	0.3 (3)
S1—N1—C4—C5	34.0 (2)	C10—C11—C12—C15	−179.53 (18)

S1—N1—C4—C3	−148.77 (14)	C11—C12—C13—C14	0.1 (3)
C3—C4—C5—C6	−0.2 (3)	C15—C12—C13—C14	179.90 (18)
N1—C4—C5—C6	177.03 (18)	C12—C13—C14—C9	−0.8 (3)
C4—C5—C6—C7	0.1 (3)	C10—C9—C14—C13	1.2 (3)
C5—C6—C7—C8	0.0 (4)	S1—C9—C14—C13	−176.68 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.87	1.89	2.640 (2)	143