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N,4-Dimethyl-*N*-phenylbenzenesulfonamide

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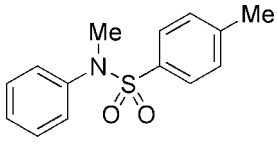
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.043; wR factor = 0.121; data-to-parameter ratio = 14.2.

The two rings in the title compound, $C_{14}H_{15}NO_2S$, are inclined to each other by an angle of 43.78 (13)°. In the crystal structure, molecules are linked by a single weak intermolecular C—H···O hydrogen bond involving an S=O group as acceptor.

Related literature

For related *N*-arylbenzenesulfonamides, see: Shi (2007); Chang *et al.* (2007); Yu *et al.* (2007); Xing *et al.* (2006); Yu (2006); Xing & Zeng (2005).



Experimental

Crystal data

$C_{14}H_{15}NO_2S$
M_r = 261.33
Monoclinic, $P2_1/n$
a = 14.156 (4) Å
b = 6.2251 (17) Å
c = 16.295 (5) Å
β = 112.821 (5)°
V = 1323.5 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.14 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.950, T_{max} = 0.968
6561 measured reflections
2341 independent reflections
1738 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.121
S = 1.04
2341 reflections
165 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 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
C11—H11···O2^{i}	0.93	2.57	3.384 (4)	147

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2144).

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supplementary materials

Acta Cryst. (2007). E**63**, o4727 [**doi:10.1107/S1600536807057650**]

N,4-Dimethyl-*N*-phenylbenzenesulfonamide

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Comment

The N atom of the title sulfonamide, (I), has a pyramidal geometry (Fig. 1), but the pyramid is somewhat shallower than expected for pure sp^3 hybridization [C9—N1—C8: 116.86 (18)°; C9—N1—S1: 117.00 (14)°; C8—N1—S1: 116.69 (15)°]. The benzene and phenyl rings are inclined to each other by an angle of 43.78 (13)°. A weak C—H···O hydrogen bond (Table 1) involving a S═O group of sulfonamide links molecules to form chains in the crystal structure. No significant π–π interactions are observed in the packing structure.

Experimental

The title compound was obtained by reaction of *N*-methylaniline with *p*-tosyl chloride in the presence of aqueous sodium biscarbonate. Colourless blocks of (I) were grown by slow evaporation of an ethyl acetate solution at 298 K.

Refinement

Methyl C atom of the *p*-tolyl group was restrained with a standard deviation of 0.01 $Å^2$ so that U_{ij} components approximate to isotropic behaviour. All H atoms were positioned geometrically (C—H = 0.93 Å for aromatic CH, 0.96 Å for methyl CH_3) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic CH and $U_{iso}(H) = 1.2U_{eq}(C)$ for methyl CH_3.

Figures

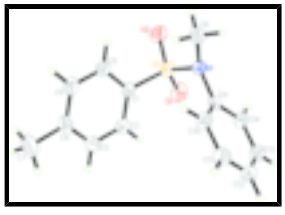

Fig. 1. The molecular structure of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids for non-H atoms.

N,4-Dimethyl-*N*-phenylbenzenesulfonamide

Crystal data

$C_{14}H_{15}NO_2S$	F_{000} = 552
M_r = 261.33	D_x = 1.312 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2238 reflections
a = 14.156 (4) Å	θ = 2.7–25.0º

b = 6.2251 (17) Å	μ = 0.24 mm^{-1}
c = 16.295 (5) Å	T = 294 (2) K
β = 112.821 (5)º	Block, colourless
V = 1323.5 (6) Å^3	0.22 × 0.20 × 0.14 mm
Z = 4	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2341 independent reflections
Radiation source: fine-focus sealed tube	1738 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −9→16
T_{min} = 0.950, T_{max} = 0.968	k = −7→7
6561 measured reflections	l = −19→14

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.043	H-atom parameters constrained
$wR(F^2)$ = 0.121	$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.4321P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
2341 reflections	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
165 parameters	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
6 restraints	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.046 (3)

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

	x	y	z	U_{iso}*/U_{eq}
S1	0.86815 (5)	0.54101 (10)	0.07849 (4)	0.0497 (2)
O1	0.83906 (15)	0.7595 (3)	0.06292 (12)	0.0671 (5)
O2	0.96603 (13)	0.4862 (3)	0.14363 (11)	0.0689 (6)
N1	0.86374 (13)	0.4405 (3)	−0.01530 (12)	0.0420 (5)
C1	0.77411 (17)	0.4082 (4)	0.10434 (14)	0.0454 (6)
C2	0.6781 (2)	0.4967 (4)	0.08104 (17)	0.0595 (7)
H2	0.6641	0.6325	0.0554	0.071*
C3	0.6033 (2)	0.3831 (5)	0.09588 (19)	0.0698 (8)
H3	0.5390	0.4449	0.0812	0.084*
C4	0.6209 (2)	0.1798 (5)	0.13204 (17)	0.0623 (7)

C5	0.7185 (2)	0.0976 (4)	0.15728 (18)	0.0623 (7)
H5	0.7331	−0.0366	0.1843	0.075*
C6	0.79442 (19)	0.2084 (4)	0.14360 (16)	0.0533 (6)
H6	0.8596	0.1491	0.1607	0.064*
C7	0.5362 (3)	0.0523 (6)	0.1427 (2)	0.0971 (11)
H7A	0.5218	0.1096	0.1912	0.146*
H7B	0.5570	−0.0951	0.1547	0.146*
H7C	0.4758	0.0608	0.0888	0.146*
C8	0.91396 (19)	0.2314 (4)	−0.01064 (18)	0.0573 (7)
H8A	0.8734	0.1205	0.0006	0.086*
H8B	0.9807	0.2338	0.0366	0.086*
H8C	0.9206	0.2035	−0.0661	0.086*
C9	0.77237 (16)	0.4813 (3)	−0.09328 (14)	0.0400 (5)
C10	0.69764 (18)	0.3281 (4)	−0.12578 (16)	0.0547 (7)
H10	0.7039	0.1977	−0.0963	0.066*
C11	0.6130 (2)	0.3688 (5)	−0.20252 (18)	0.0672 (8)
H11	0.5627	0.2640	−0.2253	0.081*
C12	0.6022 (2)	0.5600 (5)	−0.24519 (17)	0.0650 (7)
H12	0.5443	0.5871	−0.2963	0.078*
C13	0.6769 (2)	0.7121 (5)	−0.21258 (18)	0.0637 (7)
H13	0.6697	0.8432	−0.2418	0.076*
C14	0.76271 (19)	0.6736 (4)	−0.13699 (16)	0.0515 (6)
H14	0.8139	0.7771	−0.1156	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0567 (4)	0.0452 (4)	0.0430 (4)	−0.0123 (3)	0.0148 (3)	−0.0036 (3)
O1	0.1001 (14)	0.0396 (9)	0.0658 (12)	−0.0125 (9)	0.0367 (10)	−0.0088 (8)
O2	0.0501 (10)	0.0910 (14)	0.0489 (11)	−0.0176 (9)	0.0008 (8)	0.0022 (9)
N1	0.0419 (10)	0.0403 (10)	0.0425 (11)	−0.0045 (8)	0.0149 (8)	−0.0001 (8)
C1	0.0520 (14)	0.0445 (13)	0.0380 (12)	−0.0004 (10)	0.0155 (10)	−0.0003 (10)
C2	0.0616 (17)	0.0583 (16)	0.0557 (16)	0.0072 (12)	0.0195 (13)	0.0131 (12)
C3	0.0538 (17)	0.095 (2)	0.0619 (18)	0.0071 (15)	0.0239 (14)	0.0123 (16)
C4	0.0694 (18)	0.0772 (19)	0.0490 (15)	−0.0138 (15)	0.0325 (13)	−0.0015 (13)
C5	0.082 (2)	0.0521 (15)	0.0633 (17)	0.0013 (14)	0.0399 (15)	0.0081 (13)
C6	0.0588 (15)	0.0502 (14)	0.0550 (15)	0.0042 (11)	0.0266 (12)	0.0057 (11)
C7	0.090 (2)	0.122 (3)	0.098 (3)	−0.027 (2)	0.058 (2)	0.005 (2)
C8	0.0600 (16)	0.0511 (15)	0.0643 (17)	0.0055 (12)	0.0280 (13)	0.0010 (12)
C9	0.0427 (12)	0.0415 (12)	0.0385 (12)	−0.0046 (9)	0.0186 (10)	−0.0017 (9)
C10	0.0569 (15)	0.0532 (15)	0.0498 (15)	−0.0142 (12)	0.0162 (12)	0.0030 (12)
C11	0.0539 (16)	0.083 (2)	0.0584 (17)	−0.0234 (14)	0.0150 (13)	−0.0073 (15)
C12	0.0531 (16)	0.090 (2)	0.0455 (15)	0.0020 (15)	0.0118 (12)	0.0092 (15)
C13	0.0734 (18)	0.0612 (17)	0.0567 (17)	0.0089 (14)	0.0253 (14)	0.0161 (13)
C14	0.0584 (15)	0.0447 (14)	0.0511 (15)	−0.0059 (11)	0.0210 (12)	0.0029 (11)

Geometric parameters (Å, °)

S1—O1	1.4152 (18)	C7—H7A	0.9600

S1—O2	1.4219 (18)	C7—H7B	0.9600
S1—N1	1.6300 (19)	C7—H7C	0.9600
S1—C1	1.751 (2)	C8—H8A	0.9600
N1—C9	1.441 (3)	C8—H8B	0.9600
N1—C8	1.471 (3)	C8—H8C	0.9600
C1—C2	1.376 (3)	C9—C10	1.369 (3)
C1—C6	1.377 (3)	C9—C14	1.372 (3)
C2—C3	1.370 (4)	C10—C11	1.379 (3)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.378 (4)	C11—C12	1.357 (4)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.378 (4)	C12—C13	1.365 (4)
C4—C7	1.503 (4)	C12—H12	0.9300
C5—C6	1.365 (4)	C13—C14	1.375 (3)
C5—H5	0.9300	C13—H13	0.9300
C6—H6	0.9300	C14—H14	0.9300
O1—S1—O2	119.73 (11)	H7A—C7—H7B	109.5
O1—S1—N1	107.34 (10)	C4—C7—H7C	109.5
O2—S1—N1	106.24 (11)	H7A—C7—H7C	109.5
O1—S1—C1	107.52 (12)	H7B—C7—H7C	109.5
O2—S1—C1	108.60 (11)	N1—C8—H8A	109.5
N1—S1—C1	106.75 (10)	N1—C8—H8B	109.5
C9—N1—C8	116.86 (18)	H8A—C8—H8B	109.5
C9—N1—S1	117.00 (14)	N1—C8—H8C	109.5
C8—N1—S1	116.69 (15)	H8A—C8—H8C	109.5
C2—C1—C6	119.7 (2)	H8B—C8—H8C	109.5
C2—C1—S1	120.42 (19)	C10—C9—C14	120.0 (2)
C6—C1—S1	119.78 (18)	C10—C9—N1	120.9 (2)
C3—C2—C1	119.5 (2)	C14—C9—N1	119.07 (19)
C3—C2—H2	120.2	C9—C10—C11	119.5 (2)
C1—C2—H2	120.2	C9—C10—H10	120.2
C2—C3—C4	121.7 (3)	C11—C10—H10	120.2
C2—C3—H3	119.1	C12—C11—C10	120.7 (2)
C4—C3—H3	119.1	C12—C11—H11	119.6
C3—C4—C5	117.5 (2)	C10—C11—H11	119.6
C3—C4—C7	121.0 (3)	C11—C12—C13	119.6 (2)
C5—C4—C7	121.5 (3)	C11—C12—H12	120.2
C6—C5—C4	121.7 (3)	C13—C12—H12	120.2
C6—C5—H5	119.2	C12—C13—C14	120.6 (2)
C4—C5—H5	119.2	C12—C13—H13	119.7
C5—C6—C1	119.7 (2)	C14—C13—H13	119.7
C5—C6—H6	120.1	C9—C14—C13	119.5 (2)
C1—C6—H6	120.1	C9—C14—H14	120.2
C4—C7—H7A	109.5	C13—C14—H14	120.2
C4—C7—H7B	109.5		
O1—S1—N1—C9	−48.66 (18)	C3—C4—C5—C6	−2.9 (4)
O2—S1—N1—C9	−177.86 (15)	C7—C4—C5—C6	176.6 (3)
C1—S1—N1—C9	66.39 (17)	C4—C5—C6—C1	0.6 (4)

O1—S1—N1—C8	165.89 (16)	C2—C1—C6—C5	1.4 (4)
O2—S1—N1—C8	36.69 (19)	S1—C1—C6—C5	−174.82 (19)
C1—S1—N1—C8	−79.07 (18)	C8—N1—C9—C10	44.9 (3)
O1—S1—C1—C2	19.8 (2)	S1—N1—C9—C10	−100.5 (2)
O2—S1—C1—C2	150.7 (2)	C8—N1—C9—C14	−132.6 (2)
N1—S1—C1—C2	−95.2 (2)	S1—N1—C9—C14	82.0 (2)
O1—S1—C1—C6	−164.01 (19)	C14—C9—C10—C11	0.0 (4)
O2—S1—C1—C6	−33.1 (2)	N1—C9—C10—C11	−177.5 (2)
N1—S1—C1—C6	81.1 (2)	C9—C10—C11—C12	−1.1 (4)
C6—C1—C2—C3	−1.1 (4)	C10—C11—C12—C13	1.1 (4)
S1—C1—C2—C3	175.2 (2)	C11—C12—C13—C14	−0.1 (4)
C1—C2—C3—C4	−1.4 (4)	C10—C9—C14—C13	1.0 (4)
C2—C3—C4—C5	3.3 (4)	N1—C9—C14—C13	178.5 (2)
C2—C3—C4—C7	−176.2 (3)	C12—C13—C14—C9	−1.0 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O2^{i}	0.93	2.57	3.384 (4)	147

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*−1/2.

Fig. 1