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N-(3,5-Dimethylphenyl)methanesulfonamide

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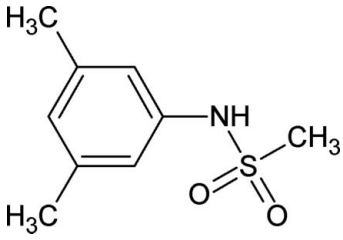
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.004 Å; R factor = 0.062; wR factor = 0.172; data-to-parameter ratio = 13.4.

The title compound, $C_9H_{13}NO_2S$, has geometric parameters similar to those of *N*-phenylmethanesulfonamide, *N*-(3-methylphenyl)methanesulfonamide, *N*-(3,5-dichlorophenyl)-methanesulfonamide and other methanesulfonanilides. The molecules in 35DMPMSA are packed into chains in the direction of the *b* axis through N—H···O hydrogen bonds and weak (methyl)C—H···O interactions.

Related literature

For related literature, see: Gowda *et al.* (2007*a*,*b*,*c*,*d*,*e*); Jayalakshmi & Gowda (2004); Klug (1968).



Experimental

Crystal data

$C_9H_{13}NO_2S$
M_r = 199.26
Monoclinic, $P2_1/c$
a = 16.273 (2) Å
b = 5.1208 (7) Å
c = 12.105 (1) Å
β = 97.84 (1)°
V = 999.3 (2) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.63 mm^{-1}
T = 299 (2) K
0.60 × 0.35 × 0.03 mm

Data collection

Enraf-Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.395, T_{max} = 0.922
2110 measured reflections
1781 independent reflections
1604 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.172
S = 1.06
1781 reflections
133 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5N···O4^{i}	0.90 (3)	2.10 (3)	2.982 (3)	168 (3)

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

Data collection: *CAD-4-PC* (Enraf-Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2408).

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supplementary materials

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N-(3,5-Dimethylphenyl)methanesulfonamide

B. T. Gowda, S. Foro and H. Fuess

Comment

The biological activity of sulfonanilides is thought to be due to the amide hydrogen portion of the molecules as it can align itself in relation to a receptor site. Thus the structural studies of sulfonanilides are of interest. In the present work, the structure of *N*-(3,5-dimethylphenyl)- methanesulfonamide has been determined as part of our study of the substituent effects on the solid state structures of methanesulfonanilides (Gowda *et al.*, 2007*a*, Gowda *et al.*, 2007*b*, Gowda *et al.*, 2007*c*, Gowda *et al.*, 2007*d*, Gowda *et al.*, 2007*e*). The structure of the title compound (Fig. 1) is similar to those of *N*-(phenyl)- methanesulfonamide (Klug, 1968), *N*-(3-methylphenyl)- methanesulfonamide (Gowda *et al.*, 2007*a*), *N*-(3,5-dichlorophenyl)-methanesulfonamide (Gowda *et al.*, 2007*e*) and other methanesulfonanilides (Gowda *et al.*, 2007*b*, *c*, *d*), with similar geometric parameters. The substitution of a methyl group at the *meta* position of PMSA (Klug, 1968) to produce 3MPMSA changes its space group from monoclinic $P2_1/c$ to orthorhombic Pccn (Gowda *et al.*, 2007*a*). The N—H···O hydrogen bonds (Table 1) build up centrosymmetric dimers (Fig. 2).

Experimental

The title compound was prepared according to the literature method (Jayalakshmi & Gowda, 2004). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Jayalakshmi & Gowda, 2004). Single crystals of the compound were obtained by slow evaporation of an ethanolic solution.

Refinement

The methyl H atoms were positioned with idealized geometry using a riding model with C—H = 0.96 Å. The other H atoms were located in difference map, and their positional parameters were refined freely [N—H = 0.90 (3) Å, and C—H = 0.89 (4)–0.99 (3) Å]. U_{iso}(H) values were set equal to 1.2 U_{eq} of the parent atom.

Figures

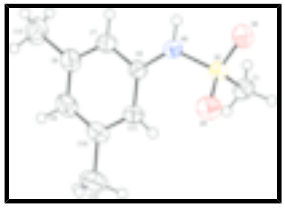

Fig. 1. Molecular structure of the title compound showing the atom labeling scheme. The displacement ellipsoids drawn at the 50% probability level.

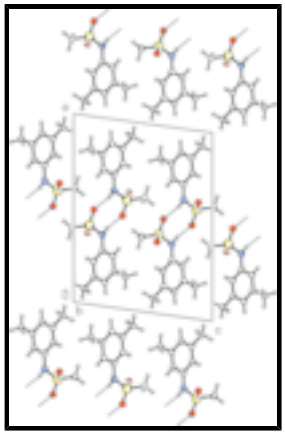

Fig. 2. Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

N-(3,5-Dimethylphenyl)methanesulfonamide

Crystal data

$C_9H_{13}NO_2S$	F_{000} = 424
M_r = 199.26	D_x = 1.324 Mg m^{-3}
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation λ = 1.54180 Å
Hall symbol: -P 2ybc	Cell parameters from 25 reflections
a = 16.273 (2) Å	θ = 7.3–37.0º
b = 5.1208 (7) Å	μ = 2.63 mm^{-1}
c = 12.105 (1) Å	T = 299 (2) K
β = 97.84 (1)º	Long plate, colourless
V = 999.3 (2) Å^3	0.60 × 0.35 × 0.03 mm
Z = 4	

Data collection

Enraf-Nonius CAD-4 diffractometer	R_{int} = 0.041
Radiation source: fine-focus sealed tube	θ_{max} = 66.9º
Monochromator: graphite	θ_{min} = 2.7º
T = 299(2) K	h = −19→19
ω/2θ scans	k = 0→6
Absorption correction: Psi-scan (North *et al.*, 1968)	l = −14→2
T_{min} = 0.395, T_{max} = 0.922	3 standard reflections
2110 measured reflections	every 120 min
1781 independent reflections	intensity decay: 1.0%
1604 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.062$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.172$	$w = 1/[\sigma^2(F_o^2) + (0.1338P)^2 + 0.2826P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.009$
1781 reflections	$\Delta\rho_{max} = 0.57$ e Å^{-3}
133 parameters	$\Delta\rho_{min} = -0.85$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2$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}
C1	0.39578 (17)	0.3450 (5)	−0.0116 (2)	0.0410 (6)
H1A	0.3368	0.3475	−0.0333	0.049*
H1B	0.4218	0.2603	−0.0685	0.049*
H1C	0.4160	0.5208	−0.0020	0.049*
C6	0.29375 (14)	0.3915 (5)	0.20981 (18)	0.0323 (5)
C7	0.27426 (16)	0.5821 (5)	0.2837 (2)	0.0386 (6)
H7	0.315 (2)	0.670 (6)	0.325 (3)	0.046*
C8	0.19292 (18)	0.6424 (5)	0.2932 (2)	0.0433 (7)
C9	0.13008 (16)	0.5109 (6)	0.2254 (3)	0.0495 (7)
H9	0.071 (2)	0.556 (7)	0.231 (3)	0.059*
C10	0.14826 (17)	0.3211 (5)	0.1507 (3)	0.0450 (7)
C11	0.23041 (15)	0.2584 (6)	0.1435 (2)	0.0390 (6)
H11	0.2410 (19)	0.125 (7)	0.097 (3)	0.047*
C12	0.1731 (2)	0.8452 (7)	0.3755 (3)	0.0632 (9)
H12A	0.1140	0.8615	0.3719	0.076*
H12B	0.1962	1.0100	0.3579	0.076*
H12C	0.1965	0.7934	0.4494	0.076*
C13	0.0797 (2)	0.1815 (8)	0.0764 (4)	0.0688 (11)
H13A	0.0319	0.2927	0.0634	0.083*
H13B	0.0655	0.0237	0.1122	0.083*
H13C	0.0983	0.1395	0.0066	0.083*

N5	0.37874 (13)	0.3388 (4)	0.20790 (17)	0.0345 (5)
H5N	0.4167 (18)	0.451 (6)	0.242 (3)	0.041*
O3	0.38043 (13)	−0.0767 (3)	0.10100 (19)	0.0510 (5)
O4	0.50638 (11)	0.1894 (4)	0.14746 (16)	0.0425 (5)
S2	0.41901 (3)	0.17442 (10)	0.11399 (4)	0.0314 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0492 (15)	0.0395 (15)	0.0339 (12)	0.0009 (11)	0.0045 (10)	0.0027 (10)
C6	0.0348 (11)	0.0303 (12)	0.0322 (11)	−0.0031 (10)	0.0059 (9)	0.0019 (9)
C7	0.0417 (13)	0.0323 (13)	0.0424 (13)	−0.0055 (10)	0.0076 (10)	−0.0028 (10)
C8	0.0470 (15)	0.0312 (14)	0.0548 (16)	−0.0005 (11)	0.0176 (12)	−0.0004 (11)
C9	0.0373 (13)	0.0450 (16)	0.0679 (18)	0.0012 (12)	0.0135 (12)	−0.0002 (14)
C10	0.0352 (13)	0.0448 (17)	0.0545 (16)	−0.0063 (11)	0.0038 (11)	0.0000 (12)
C11	0.0392 (13)	0.0360 (13)	0.0417 (13)	−0.0066 (11)	0.0057 (10)	−0.0069 (12)
C12	0.066 (2)	0.050 (2)	0.080 (2)	0.0001 (15)	0.0325 (18)	−0.0163 (16)
C13	0.0410 (15)	0.074 (3)	0.088 (3)	−0.0103 (15)	−0.0026 (15)	−0.0183 (19)
N5	0.0334 (10)	0.0351 (12)	0.0348 (10)	−0.0034 (8)	0.0038 (8)	−0.0058 (8)
O3	0.0642 (13)	0.0204 (10)	0.0702 (13)	−0.0042 (8)	0.0153 (9)	−0.0027 (8)
O4	0.0390 (11)	0.0408 (11)	0.0486 (11)	0.0099 (7)	0.0089 (8)	0.0058 (8)
S2	0.0361 (4)	0.0226 (4)	0.0361 (4)	0.00312 (19)	0.0064 (3)	0.00110 (19)

Geometric parameters (Å, °)

C1—S2	1.750 (2)	C10—C11	1.389 (4)
C1—H1A	0.9600	C10—C13	1.513 (4)
C1—H1B	0.9600	C11—H11	0.92 (3)
C1—H1C	0.9600	C12—H12A	0.9600
C6—C7	1.390 (4)	C12—H12B	0.9600
C6—C11	1.395 (4)	C12—H12C	0.9600
C6—N5	1.412 (3)	C13—H13A	0.9600
C7—C8	1.379 (4)	C13—H13B	0.9600
C7—H7	0.89 (4)	C13—H13C	0.9600
C8—C9	1.394 (4)	N5—S2	1.623 (2)
C8—C12	1.505 (4)	N5—H5N	0.90 (3)
C9—C10	1.387 (4)	O3—S2	1.4300 (19)
C9—H9	0.99 (3)	O4—S2	1.4262 (19)
S2—C1—H1A	109.5	C6—C11—H11	122.1 (19)
S2—C1—H1B	109.5	C8—C12—H12A	109.5
H1A—C1—H1B	109.5	C8—C12—H12B	109.5
S2—C1—H1C	109.5	H12A—C12—H12B	109.5
H1A—C1—H1C	109.5	C8—C12—H12C	109.5
H1B—C1—H1C	109.5	H12A—C12—H12C	109.5
C7—C6—C11	119.9 (2)	H12B—C12—H12C	109.5
C7—C6—N5	117.0 (2)	C10—C13—H13A	109.5
C11—C6—N5	123.1 (2)	C10—C13—H13B	109.5
C8—C7—C6	121.1 (2)	H13A—C13—H13B	109.5

C8—C7—H7	119 (2)	C10—C13—H13C	109.5
C6—C7—H7	120 (2)	H13A—C13—H13C	109.5
C7—C8—C9	118.6 (3)	H13B—C13—H13C	109.5
C7—C8—C12	120.3 (3)	C6—N5—S2	126.90 (17)
C9—C8—C12	121.1 (3)	C6—N5—H5N	118.8 (19)
C10—C9—C8	121.2 (2)	S2—N5—H5N	109.6 (19)
C10—C9—H9	120 (2)	O4—S2—O3	119.03 (11)
C8—C9—H9	119 (2)	O4—S2—N5	104.79 (11)
C9—C10—C11	119.7 (2)	O3—S2—N5	109.27 (12)
C9—C10—C13	120.9 (3)	O4—S2—C1	107.99 (12)
C11—C10—C13	119.4 (3)	O3—S2—C1	108.29 (13)
C10—C11—C6	119.5 (3)	N5—S2—C1	106.85 (12)
C10—C11—H11	118.3 (19)		
C11—C6—C7—C8	0.2 (4)	C13—C10—C11—C6	178.4 (3)
N5—C6—C7—C8	−178.5 (2)	C7—C6—C11—C10	1.0 (4)
C6—C7—C8—C9	−1.1 (4)	N5—C6—C11—C10	179.7 (2)
C6—C7—C8—C12	178.6 (3)	C7—C6—N5—S2	−166.20 (19)
C7—C8—C9—C10	0.7 (4)	C11—C6—N5—S2	15.1 (3)
C12—C8—C9—C10	−179.0 (3)	C6—N5—S2—O4	177.13 (19)
C8—C9—C10—C11	0.5 (4)	C6—N5—S2—O3	−54.3 (2)
C8—C9—C10—C13	−179.3 (3)	C6—N5—S2—C1	62.7 (2)
C9—C10—C11—C6	−1.4 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5N···O4^{i}	0.90 (3)	2.10 (3)	2.982 (3)	168 (3)

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

Fig. 1

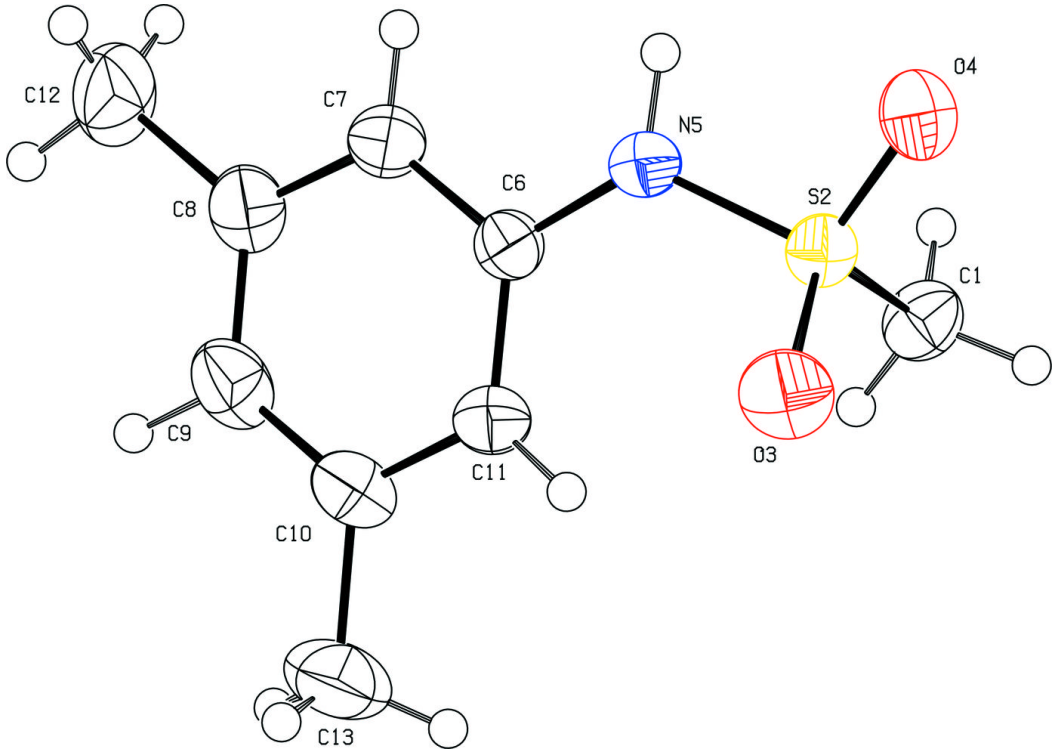

Fig. 2