

N-(2,4,6-Trimethylphenyl)methanesulfonamide

 B. Thimme Gowda,^{a*} Sabine Foro^b and Hartmut Fuess^b

^aDepartment of Chemistry, Mangalore University, Mangalagangothri 574 199, Mangalore, India, and ^bInstitute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany

Correspondence e-mail: gowdabt@yahoo.com

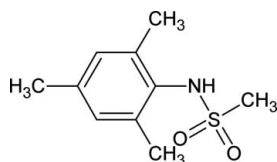
Received 25 May 2007; accepted 28 May 2007

Key indicators: single-crystal X-ray study; $T = 299$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.069; wR factor = 0.198; data-to-parameter ratio = 14.9.

The structure of the title compound, $\text{C}_{10}\text{H}_{15}\text{NO}_2\text{S}$, resembles those of other methanesulfonamides, with similar geometric parameters except for some differences in the bond and torsion angles. The amide H atom lies on one side of the plane of the benzene ring, while the methanesulfonyl group is on the opposite side of the plane, as in other methanesulfonamides. The amide H atom is thus available to a receptor molecule during its biological activity. The molecules are packed into polymeric chains in the direction of the b axis through $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2007*a,b,c,d,e,f,g,h,i,j,k,l,m,n*); Jayalakshmi & Gowda (2004); Klug (1968).



Experimental

Crystal data

 $\text{C}_{10}\text{H}_{15}\text{NO}_2\text{S}$
 $M_r = 213.29$

 Monoclinic, $P2_1/n$
 $a = 14.588$ (4) Å

 $b = 4.920$ (2) Å

 $c = 16.386$ (8) Å

 $\beta = 111.49$ (9)°

 $V = 1094.3$ (8) Å³
 $Z = 4$

 Cu $K\alpha$ radiation

 $\mu = 2.43$ mm⁻¹
 $T = 299$ (2) K

 $0.60 \times 0.11 \times 0.03$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer

 Absorption correction: ψ scan (North *et al.*, 1968)

 $T_{\min} = 0.701$, $T_{\max} = 0.996$ (expected range = 0.654–0.930)

2261 measured reflections

1953 independent reflections

 1385 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.114$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.069$
 $wR(F^2) = 0.198$
 $S = 1.02$

1953 reflections

 3 standard reflections
 frequency: 120 min
 intensity decay: 1.2%

131 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.84$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.55$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N5}-\text{H5}\cdots\text{O4}^i$	0.86	2.33	2.944 (4)	128

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

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: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

BTG gratefully thanks the Alexander von Humboldt Foundation, Bonn, Germany, for extensions of his research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2182).

References

- Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
- Enraf–Nonius (1996). *CAD-4-PC*. Version 2.0. Enraf–Nonius, Delft, The Netherlands.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*a*). *Acta Cryst.* **E63**, o2337.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*b*). *Acta Cryst.* **E63**, o2338.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*c*). *Acta Cryst.* **E63**, o2339.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*d*). *Acta Cryst.* **E63**, o2340.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*e*). *Acta Cryst.* **E63**, o2569.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*f*). *Acta Cryst.* **E63**, o2570.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*g*). *Acta Cryst.* **E63**, o2597.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*h*). *Acta Cryst.* **E63**, o3014.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*i*). *Acta Cryst.* **E63**, o3015.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*j*). *Acta Cryst.* **E63**, o3085.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*k*). *Acta Cryst.* **E63**, o3086.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*l*). *Acta Cryst.* **E63**, o3087.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*m*). *Acta Cryst.* **E63**, o3088 o3089.
- Gowda, B. T., Foro, S. & Fuess, H. (2007*n*). In preparation.
- Jayalakshmi, K. L. & Gowda, B. T. (2004). *Z. Naturforsch. Teil A*, **59**, 491–500.
- Klug, H. P. (1968). *Acta Cryst.* **B24**, 792–802.
- North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Stoe & Cie (1987). *REDU4*. Stoe & Cie GmbH, Darmstadt, Germany.

supplementary materials

Acta Cryst. (2007). E63, o3084 [doi:10.1107/S1600536807025883]

N-(2,4,6-Trimethylphenyl)methanesulfonamide

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

Comment

The biological activity of alkyl sulphonanilides is thought to be due to the hydrogen of the phenyl N—H portion of the sulphonanilide molecules as it can align itself, in relation to a receptor site. Therefore the structural studies of sulphonanilides are of interest. In the present work, the structure of *N*-(2,4,6-trimethylphenyl)-methanesulfonamide (246TMPMSA) has been determined to explore the substituent effects on the solid state structures of sulfonanilides (Gowda *et al.*, 2007*a,b,c,d,e,f,g,h,i,j,k,l,m,n*). The structure of 246TMPMSA (Fig. 1) resembles those of *N*-(phenyl)-methanesulfonamide (PMSA) (Klug, 1968), *N*-(2-methylphenyl)-methanesulfonamide (2MPMSA), *N*-(4-methylphenyl)-methanesulfonamide (4MPMSA), *N*-(2,4-dimethylphenyl)-methanesulfonamide (24DMPMSA), *N*-(2,6-dimethylphenyl)-methanesulfonamide (26DMPMSA) and other methanesulfonanilides (Gowda *et al.*, 2007*a,b,c,d,e,f,g,h,i,j,k, l,m,n*). The *ortho* substitution of a methyl group in PMSA changes its space group from monoclinic $P2_1/c$ (Klug, 1968) to triclinic P-1 (Gowda *et al.*, 2007*d*). The substitution of an additional methyl group at the second *ortho* position in 2MPMSA to produce 26DMPMSA changes the space group from triclinic P-1 to orthorhombic $P2_12_12_1$, determined under identical conditions (Gowda *et al.*, 2007*n*). Introduction of the third methyl group at the *para* position of 26DMPMSA to produce 246TMPMSA changes the space group from orthorhombic $P2_12_12_1$ to monoclinic $P2_1/n$. The geometric parameters in 246TMPMSA are similar to those in PMSA, 2MPMSA, 4MPMSA, 24DMPMSA, 26DMPMSA and other methanesulfonanilides (Gowda *et al.*, 2007*a-n*), except for some difference in the bond and torsional angles. The amide hydrogen sits alone on one side of the plane of the phenyl group, while the whole methanesulfonyl group is on the opposite side of the plane, similar to that in other methanesulfonanilides. The amide hydrogen is thus available to a receptor molecule during its biological activity. The molecules in 246TMPMSA are packed into polymeric chain in the direction of *b* axis through N—H \cdots O hydrogen bonds (Fig. 2, Table 1).

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 title compound were obtained from a slow evaporation of its ethanolic solution and used for X-ray diffraction studied at room temperature.

Refinement

All H atoms attached were fixed geometrically and treated as riding on their parent atoms with C—H = 0.93 Å (C_{aromatic}) or 0.96 Å (CH_3) and N—H = 0.86 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(C_{\text{aromatic}} \text{ or } \text{N})$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{CH}_3)$.

Figures

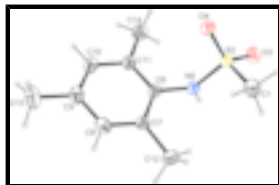


Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

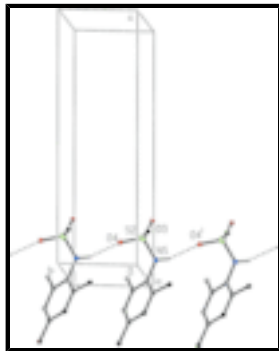


Fig. 2. Partial packing view of the title compound showing the formation of chain parallel to the *b* axis through N—H...O hydrogen bonds axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bondings have been omitted for clarity. [Symmetry code: (i) *x*, *y* - 1, *z*].

N-(2,4,6-Trimethylphenyl)methanesulfonamide

Crystal data

$C_{10}H_{15}NO_2S$

$M_r = 213.29$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 14.588$ (4) Å

$b = 4.920$ (2) Å

$c = 16.386$ (8) Å

$\beta = 111.49$ (9)°

$V = 1094.3$ (8) Å³

$Z = 4$

$F_{000} = 456$

$D_x = 1.295$ Mg m⁻³

Cu $K\alpha$ radiation

$\lambda = 1.54180$ Å

Cell parameters from 25 reflections

$\theta = 7.0$ – 19.1 °

$\mu = 2.43$ mm⁻¹

$T = 299$ (2) K

Needle, colourless

$0.60 \times 0.11 \times 0.03$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 299$ (2) K

ω/θ scans

Absorption correction: Psi-scan
(North *et al.*, 1968)

$T_{\min} = 0.701$, $T_{\max} = 0.996$

2261 measured reflections

1953 independent reflections

$R_{\text{int}} = 0.114$

$\theta_{\text{max}} = 67.0$ °

$\theta_{\text{min}} = 3.5$ °

$h = -17 \rightarrow 2$

$k = 0 \rightarrow 5$

$l = -18 \rightarrow 19$

3 standard reflections

every 120 min

intensity decay: 1.2%

1385 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
$R[F^2 > 2\sigma(F^2)] = 0.069$	H-atom parameters constrained
$wR(F^2) = 0.198$	$w = 1/[\sigma^2(F_o^2) + (0.1367P)^2]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
1953 reflections	$(\Delta/\sigma)_{\max} = 0.031$
131 parameters	$\Delta\rho_{\max} = 0.84 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.55 \text{ e } \text{\AA}^{-3}$
	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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1583 (3)	-0.1041 (11)	0.1477 (3)	0.0605 (12)
H1A	0.1547	-0.2978	0.1528	0.091*
H1B	0.1020	-0.0415	0.0993	0.091*
H1C	0.1590	-0.0197	0.2008	0.091*
C6	0.2181 (3)	-0.0825 (7)	-0.0439 (2)	0.0366 (8)
C7	0.1251 (3)	-0.1758 (7)	-0.0963 (2)	0.0395 (9)
C8	0.0818 (3)	-0.0731 (8)	-0.1804 (2)	0.0455 (9)
H8	0.0206	-0.1397	-0.2163	0.055*
C9	0.1265 (3)	0.1260 (9)	-0.2131 (2)	0.0487 (10)
C10	0.2200 (3)	0.2072 (10)	-0.1605 (3)	0.0489 (10)
H10	0.2523	0.3342	-0.1824	0.059*
C11	0.2685 (3)	0.1074 (8)	-0.0758 (2)	0.0408 (9)
C12	0.0716 (3)	-0.3944 (9)	-0.0663 (3)	0.0541 (11)
H12A	0.0219	-0.4751	-0.1164	0.081*
H12B	0.0412	-0.3153	-0.0289	0.081*
H12C	0.1177	-0.5314	-0.0344	0.081*
C13	0.0751 (4)	0.2409 (12)	-0.3028 (3)	0.0710 (14)

supplementary materials

H13A	0.0371	0.3965	-0.2991	0.107*
H13B	0.0322	0.1058	-0.3396	0.107*
H13C	0.1229	0.2943	-0.3272	0.107*
C14	0.3723 (3)	0.1976 (10)	-0.0241 (3)	0.0567 (11)
H14A	0.4035	0.2541	-0.0637	0.085*
H14B	0.4086	0.0493	0.0112	0.085*
H14C	0.3710	0.3469	0.0132	0.085*
N5	0.2665 (2)	-0.1810 (6)	0.04429 (19)	0.0405 (8)
H5	0.2971	-0.3338	0.0518	0.049*
O3	0.3461 (2)	-0.1205 (6)	0.20308 (18)	0.0558 (8)
O4	0.2624 (3)	0.2640 (6)	0.1099 (2)	0.0637 (10)
S2	0.26621 (7)	-0.01834 (17)	0.12998 (5)	0.0394 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.067 (3)	0.066 (3)	0.057 (3)	-0.002 (2)	0.033 (2)	-0.007 (2)
C6	0.048 (2)	0.0289 (17)	0.0370 (17)	0.0049 (15)	0.0202 (16)	0.0029 (14)
C7	0.050 (2)	0.0295 (19)	0.044 (2)	-0.0014 (15)	0.0229 (17)	-0.0048 (15)
C8	0.044 (2)	0.049 (2)	0.0422 (19)	0.0018 (17)	0.0133 (16)	-0.0092 (18)
C9	0.056 (2)	0.055 (3)	0.0374 (19)	0.0074 (19)	0.0198 (18)	-0.0003 (18)
C10	0.059 (3)	0.051 (2)	0.044 (2)	0.0020 (19)	0.0288 (19)	0.0101 (18)
C11	0.045 (2)	0.042 (2)	0.0373 (18)	0.0007 (16)	0.0181 (16)	0.0024 (16)
C12	0.058 (3)	0.046 (2)	0.063 (3)	-0.0145 (19)	0.027 (2)	-0.004 (2)
C13	0.079 (3)	0.087 (4)	0.043 (2)	0.020 (3)	0.018 (2)	0.012 (2)
C14	0.052 (3)	0.065 (3)	0.056 (2)	-0.006 (2)	0.024 (2)	0.005 (2)
N5	0.062 (2)	0.0245 (15)	0.0372 (16)	0.0087 (13)	0.0206 (14)	0.0038 (12)
O3	0.0647 (19)	0.0549 (19)	0.0417 (15)	0.0019 (14)	0.0122 (13)	0.0032 (13)
O4	0.128 (3)	0.0200 (15)	0.0497 (17)	0.0024 (14)	0.0397 (18)	0.0021 (12)
S2	0.0600 (6)	0.0242 (5)	0.0340 (5)	0.0010 (4)	0.0173 (4)	0.0033 (3)

Geometric parameters (\AA , $^\circ$)

C1—S2	1.754 (4)	C11—C14	1.506 (6)
C1—H1A	0.9600	C12—H12A	0.9600
C1—H1B	0.9600	C12—H12B	0.9600
C1—H1C	0.9600	C12—H12C	0.9600
C6—C7	1.391 (5)	C13—H13A	0.9600
C6—C11	1.402 (5)	C13—H13B	0.9600
C6—N5	1.440 (4)	C13—H13C	0.9600
C7—C8	1.385 (5)	C14—H14A	0.9600
C7—C12	1.513 (5)	C14—H14B	0.9600
C8—C9	1.388 (6)	C14—H14C	0.9600
C8—H8	0.9300	N5—S2	1.618 (3)
C9—C10	1.379 (6)	N5—H5	0.8600
C9—C13	1.494 (6)	O3—S2	1.422 (3)
C10—C11	1.396 (5)	O4—S2	1.424 (3)
C10—H10	0.9300		

S2—C1—H1A	109.5	H12A—C12—H12B	109.5
S2—C1—H1B	109.5	C7—C12—H12C	109.5
H1A—C1—H1B	109.5	H12A—C12—H12C	109.5
S2—C1—H1C	109.5	H12B—C12—H12C	109.5
H1A—C1—H1C	109.5	C9—C13—H13A	109.5
H1B—C1—H1C	109.5	C9—C13—H13B	109.5
C7—C6—C11	121.1 (3)	H13A—C13—H13B	109.5
C7—C6—N5	121.1 (3)	C9—C13—H13C	109.5
C11—C6—N5	117.8 (3)	H13A—C13—H13C	109.5
C8—C7—C6	118.7 (4)	H13B—C13—H13C	109.5
C8—C7—C12	118.8 (4)	C11—C14—H14A	109.5
C6—C7—C12	122.5 (3)	C11—C14—H14B	109.5
C7—C8—C9	122.3 (4)	H14A—C14—H14B	109.5
C7—C8—H8	118.9	C11—C14—H14C	109.5
C9—C8—H8	118.9	H14A—C14—H14C	109.5
C10—C9—C8	117.4 (4)	H14B—C14—H14C	109.5
C10—C9—C13	122.1 (4)	C6—N5—S2	123.3 (3)
C8—C9—C13	120.5 (4)	C6—N5—H5	118.4
C9—C10—C11	123.0 (4)	S2—N5—H5	118.4
C9—C10—H10	118.5	O3—S2—O4	119.3 (2)
C11—C10—H10	118.5	O3—S2—N5	107.10 (19)
C10—C11—C6	117.4 (4)	O4—S2—N5	107.14 (17)
C10—C11—C14	119.7 (4)	O3—S2—C1	106.5 (2)
C6—C11—C14	122.9 (3)	O4—S2—C1	108.1 (2)
C7—C12—H12A	109.5	N5—S2—C1	108.3 (2)
C7—C12—H12B	109.5		

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N5—H5 \cdots O4 ⁱ	0.86	2.33	2.944 (4)	128

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

Fig. 1

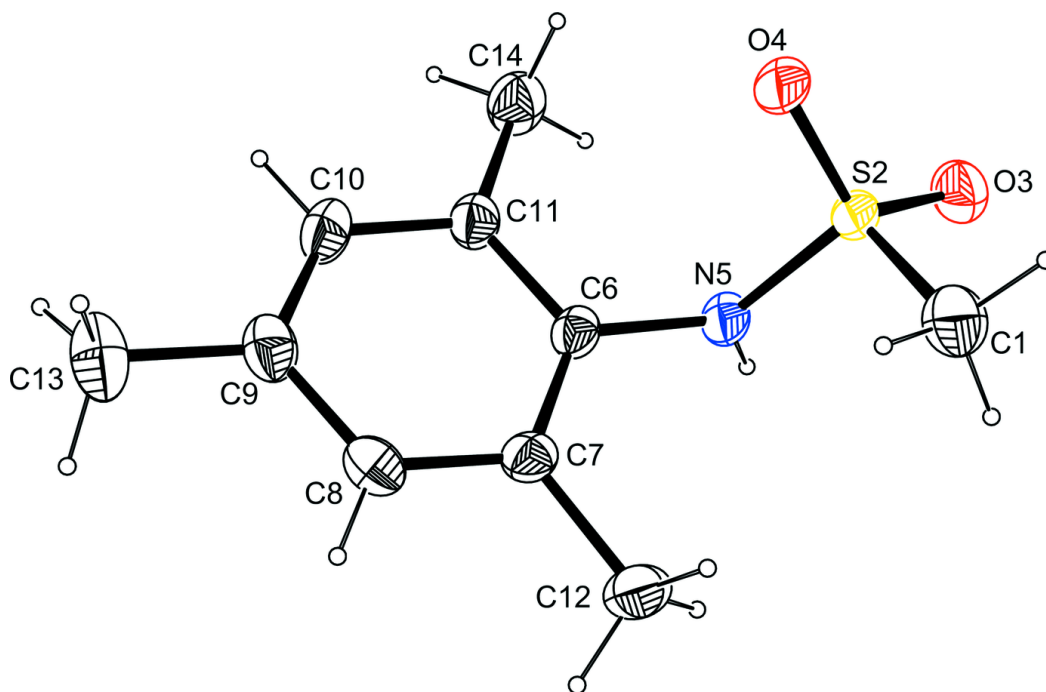


Fig. 2

