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2,2-Dimethyl-*N*-(phenylsulfonyl)-acetamide

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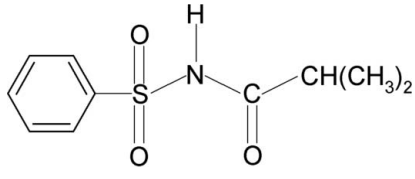
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.007 Å; R factor = 0.073; wR factor = 0.213; data-to-parameter ratio = 14.8.

In the title compound, $C_{10}H_{13}NO_3S$, the N—H and C═O bonds in the SO_2—NH—CO—C segment are *anti* to each other. The benzene ring and the SO_2—NH—CO—C segment form a dihedral angle of 87.4 (1)°. The crystal packing features inversion-related dimers linked by pairs of N—H···O hydrogen bonds.

Related literature

For sulfonamide drugs, see: Maren (1976). It has been postulated that the propensity for hydrogen bonding in the solid state can give rise to polymorphism due to the presence of various hydrogen-bond donors and acceptors, see: Yang & Guillory (1972). The hydrogen bonding preferences of sulfonamides have also been investigated, see: Adsmond & Grant (2001). The nature and position of substituents play a significant role in the crystal structures of *N*-(aryl)sulfonoamides, see: Gowda *et al.* (2008*a*,*b*,*c*);



Experimental

Crystal data

$C_{10}H_{13}NO_3S$ M_r = 227.27
Monoclinic, $P2_1/c$
a = 6.1240 (4) Å
b = 22.201 (2) Å
c = 8.9192 (9) Å
β = 106.903 (6)°
V = 1160.26 (17) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.40 mm^{-1}
T = 299 K
0.50 × 0.13 × 0.08 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
2732 measured reflections
2075 independent reflections
1755 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.213
S = 1.08
2075 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O2^{i}	0.81 (4)	2.12 (5)	2.898 (4)	160 (4)

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

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, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); 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: FL2270).

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supplementary materials

Acta Cryst. (2009). E**65**, o2680 [**doi:10.1107/S1600536809040483**]

2,2-Dimethyl-*N*-(phenylsulfonyl)acetamide

B. T. Gowda, S. Foro, P. G. Nirmala and H. Fuess

Comment

Sulfonamide drugs that exhibit antibacterial activity contain the sulfanilamide moiety (Maren, 1976). It has been postulated that the propensity for hydrogen bonding in the solid state, due to the presence of various hydrogen bond donors and acceptors, can give rise to polymorphism (Yang & Guillory, 1972). The hydrogen bonding preferences of sulfonamides have also been investigated (Adsmond & Grant, 2001). The nature and position of substituents play a significant role in the crystal structures of *N*-(aryl)sulfonoamides (Gowda *et al.*, 2008*a, b, c*).

As part of our substituent effect studies, the structure of (I) has been determined. The N—H and C=O bonds of the SO_2—NH—CO—C segment in (I) are anti to each other (Fig. 1), similar to that observed in *N*-(phenylsulfonyl)2,2,2-trimethylacetamide (II)(Gowda *et al.*, 2008*c*), *N*-(phenylsulfonyl)2,2-dichloroacetamide (III) (Gowda *et al.*, 2008*a*) and other sulfonoamides (Gowda *et al.*, 2008*b*). The SO_2—NH—CO—C segment forms a dihedral angle of 87.4 (1)° with the benzene ring, compared to values of 83.2 (1) and 76.0 (1)° (for the two independent molecules of (II)) and 79.8 (1)° in (III). In the crystal the molecules form inversion-related dimers along the *c* axis, linked by pairs of N—H···O(S) hydrogen bonds (Table 1, Fig.2).

Experimental

The title compound was prepared by refluxing benzenesulfonamide (0.10 mole) with an excess of isobutanoyl chloride (0.20 mole) for about an hour on a water bath. The reaction mixture was cooled and poured into ice cold water. The resulting solid was separated, washed thoroughly with water and dissolved in warm dilute sodium hydrogen carbonate solution. The title compound was reprecipitated by acidifying the filtered solution with glacial acetic acid. It was filtered, dried and recrystallized from ethanol. The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared spectra. Single crystals of the title compound used for X-ray diffraction studies were obtained from a slow evaporation of an ethanolic solution of the compound.

Refinement

The H atom of the NH group was located in a difference map and and its position refined with N—H = 0.81 (4) Å. The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93–0.98 Å.

All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom).

Figures

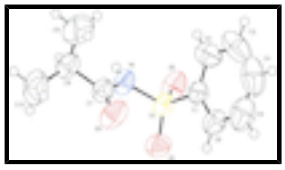

Fig. 1. Molecular structure of (I), showing the atom labeling scheme. The displacement ellipsoids are drawn at the 50% probability level. The H atoms are represented as small spheres of arbitrary radii.

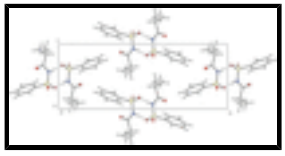

Fig. 2. Molecular packing of (I) with hydrogen bonding shown as dashed lines.

2,2-Dimethyl-*N*-(phenylsulfonyl)acetamide

Crystal data

$C_{10}H_{13}NO_3S$	F_{000} = 480
M_r = 227.27	D_x = 1.301 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 = 6.1240 (4) Å	θ = 4.0–20.3º
b = 22.201 (2) Å	μ = 2.40 mm^{-1}
c = 8.9192 (9) Å	T = 299 K
β = 106.903 (6)º	Rod, colourless
V = 1160.26 (17) Å^3	0.50 × 0.13 × 0.08 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.047
Radiation source: fine-focus sealed tube	θ_{max} = 67.0º
Monochromator: graphite	θ_{min} = 4.0º
T = 299 K	h = 0→7
ω/2θ scans	k = −26→4
Absorption correction: none	l = −10→10
2732 measured reflections	3 standard reflections
2075 independent reflections	every 120 min
1755 reflections with $I > 2\sigma(I)$	intensity decay: 1.0%

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.073	$w = 1/[\sigma^2(F_o^2) + (0.1492P)^2 + 0.3098P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.213$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.08$	$\Delta\rho_{max} = 0.78$ e Å^{-3}
2075 reflections	$\Delta\rho_{min} = -0.58$ e Å^{-3}
140 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.029 (4)
Secondary atom site location: difference Fourier map	

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 $F^2 > \sigma(F^2)$ 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	0.4133 (5)	0.36281 (13)	0.1597 (3)	0.0566 (7)
C2	0.6038 (6)	0.3479 (2)	0.1164 (5)	0.0806 (10)
H2	0.6706	0.3751	0.0637	0.097*
C3	0.6932 (8)	0.2901 (3)	0.1549 (7)	0.1103 (19)
H3	0.8212	0.2782	0.1263	0.132*
C4	0.5957 (12)	0.2509 (2)	0.2337 (7)	0.117 (2)
H4	0.6587	0.2128	0.2591	0.141*
C5	0.4070 (11)	0.26677 (19)	0.2757 (6)	0.1049 (15)
H5	0.3418	0.2397	0.3297	0.126*
C6	0.3138 (7)	0.32271 (16)	0.2382 (4)	0.0734 (9)
H6	0.1838	0.3337	0.2655	0.088*
C7	0.0475 (5)	0.41022 (15)	−0.1737 (4)	0.0627 (8)
C8	0.0133 (7)	0.42667 (17)	−0.3429 (4)	0.0721 (9)
H8	0.0582	0.4689	−0.3459	0.087*
C9	0.1661 (13)	0.3903 (4)	−0.4061 (7)	0.162 (3)
H9A	0.1324	0.3484	−0.3988	0.194*
H9B	0.3216	0.3980	−0.3470	0.194*
H9C	0.1443	0.4008	−0.5139	0.194*
C10	−0.2332 (10)	0.4217 (3)	−0.4352 (6)	0.123 (2)
H10A	−0.3227	0.4479	−0.3908	0.148*
H10B	−0.2835	0.3809	−0.4321	0.148*
H10C	−0.2514	0.4332	−0.5420	0.148*
N1	0.2199 (5)	0.44210 (13)	−0.0704 (3)	0.0632 (8)

H1N	0.280 (7)	0.4703 (19)	−0.101 (5)	0.076*
O1	0.1032 (5)	0.43906 (11)	0.1775 (3)	0.0754 (7)
O2	0.4768 (5)	0.47818 (11)	0.1727 (3)	0.0779 (8)
O3	−0.0530 (5)	0.37102 (14)	−0.1283 (3)	0.0923 (10)
S1	0.29657 (13)	0.43493 (3)	0.12050 (8)	0.0570 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0624 (17)	0.0556 (16)	0.0489 (15)	−0.0002 (12)	0.0118 (13)	−0.0021 (11)
C2	0.0643 (19)	0.094 (3)	0.084 (2)	−0.0031 (18)	0.0227 (17)	−0.020 (2)
C3	0.074 (3)	0.120 (4)	0.122 (4)	0.030 (3)	0.005 (3)	−0.043 (3)
C4	0.137 (5)	0.080 (3)	0.105 (4)	0.038 (3)	−0.012 (3)	−0.005 (3)
C5	0.144 (4)	0.071 (2)	0.094 (3)	0.014 (3)	0.026 (3)	0.021 (2)
C6	0.090 (2)	0.0648 (19)	0.0673 (19)	0.0021 (17)	0.0261 (17)	0.0103 (15)
C7	0.0627 (17)	0.0669 (18)	0.0547 (17)	−0.0113 (14)	0.0112 (14)	0.0026 (13)
C8	0.083 (2)	0.076 (2)	0.0534 (18)	−0.0139 (17)	0.0147 (16)	−0.0006 (15)
C9	0.184 (7)	0.226 (8)	0.096 (4)	0.083 (6)	0.074 (4)	0.015 (5)
C10	0.113 (4)	0.163 (5)	0.068 (3)	−0.016 (3)	−0.015 (3)	0.003 (3)
N1	0.0731 (17)	0.0619 (16)	0.0497 (14)	−0.0170 (12)	0.0104 (12)	0.0071 (11)
O1	0.0876 (17)	0.0760 (16)	0.0715 (15)	0.0129 (12)	0.0370 (13)	0.0004 (11)
O2	0.0986 (18)	0.0689 (14)	0.0570 (13)	−0.0292 (12)	0.0081 (12)	−0.0041 (10)
O3	0.0977 (19)	0.108 (2)	0.0663 (15)	−0.0501 (16)	0.0162 (13)	0.0048 (13)
S1	0.0701 (6)	0.0519 (5)	0.0477 (5)	−0.0063 (3)	0.0153 (4)	−0.0007 (3)

Geometric parameters (Å, °)

C1—C2	1.372 (5)	C7—C8	1.507 (4)
C1—C6	1.379 (5)	C8—C9	1.466 (7)
C1—S1	1.747 (3)	C8—C10	1.499 (6)
C2—C3	1.400 (7)	C8—H8	0.9800
C2—H2	0.9300	C9—H9A	0.9600
C3—C4	1.361 (8)	C9—H9B	0.9600
C3—H3	0.9300	C9—H9C	0.9600
C4—C5	1.361 (8)	C10—H10A	0.9600
C4—H4	0.9300	C10—H10B	0.9600
C5—C6	1.367 (6)	C10—H10C	0.9600
C5—H5	0.9300	N1—S1	1.637 (3)
C6—H6	0.9300	N1—H1N	0.81 (4)
C7—O3	1.202 (4)	O1—S1	1.420 (3)
C7—N1	1.378 (4)	O2—S1	1.435 (2)
C2—C1—C6	121.7 (3)	C9—C8—H8	107.5
C2—C1—S1	119.7 (3)	C10—C8—H8	107.5
C6—C1—S1	118.6 (3)	C7—C8—H8	107.5
C1—C2—C3	117.1 (4)	C8—C9—H9A	109.5
C1—C2—H2	121.4	C8—C9—H9B	109.5
C3—C2—H2	121.4	H9A—C9—H9B	109.5
C4—C3—C2	121.0 (4)	C8—C9—H9C	109.5

C4—C3—H3	119.5	H9A—C9—H9C	109.5
C2—C3—H3	119.5	H9B—C9—H9C	109.5
C5—C4—C3	120.8 (4)	C8—C10—H10A	109.5
C5—C4—H4	119.6	C8—C10—H10B	109.5
C3—C4—H4	119.6	H10A—C10—H10B	109.5
C4—C5—C6	119.7 (5)	C8—C10—H10C	109.5
C4—C5—H5	120.1	H10A—C10—H10C	109.5
C6—C5—H5	120.1	H10B—C10—H10C	109.5
C5—C6—C1	119.7 (4)	C7—N1—S1	125.3 (2)
C5—C6—H6	120.1	C7—N1—H1N	120 (3)
C1—C6—H6	120.1	S1—N1—H1N	114 (3)
O3—C7—N1	120.9 (3)	O1—S1—O2	118.90 (16)
O3—C7—C8	125.3 (3)	O1—S1—N1	110.43 (16)
N1—C7—C8	113.7 (3)	O2—S1—N1	103.49 (14)
C9—C8—C10	113.7 (5)	O1—S1—C1	108.82 (15)
C9—C8—C7	109.5 (4)	O2—S1—C1	108.49 (16)
C10—C8—C7	110.9 (4)	N1—S1—C1	105.91 (14)
C6—C1—C2—C3	0.2 (5)	O3—C7—N1—S1	−4.4 (5)
S1—C1—C2—C3	178.2 (3)	C8—C7—N1—S1	179.4 (3)
C1—C2—C3—C4	−0.8 (7)	C7—N1—S1—O1	−50.6 (3)
C2—C3—C4—C5	0.6 (8)	C7—N1—S1—O2	−178.9 (3)
C3—C4—C5—C6	0.2 (8)	C7—N1—S1—C1	67.1 (3)
C4—C5—C6—C1	−0.8 (7)	C2—C1—S1—O1	−179.6 (3)
C2—C1—C6—C5	0.6 (6)	C6—C1—S1—O1	−1.4 (3)
S1—C1—C6—C5	−177.5 (3)	C2—C1—S1—O2	−48.8 (3)
O3—C7—C8—C9	−88.9 (6)	C6—C1—S1—O2	129.3 (3)
N1—C7—C8—C9	87.0 (5)	C2—C1—S1—N1	61.7 (3)
O3—C7—C8—C10	37.3 (6)	C6—C1—S1—N1	−120.1 (3)
N1—C7—C8—C10	−146.7 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O2^{i}	0.81 (4)	2.12 (5)	2.898 (4)	160 (4)

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

Fig. 1

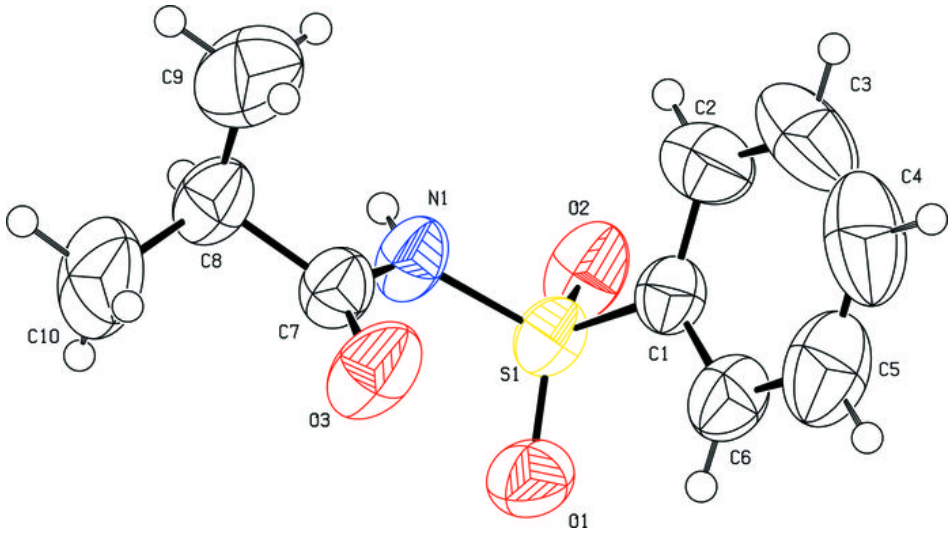

Fig. 2