

## (E)-2-Methyl-N-[4-(methylsulfonyl)-benzylidene]aniline

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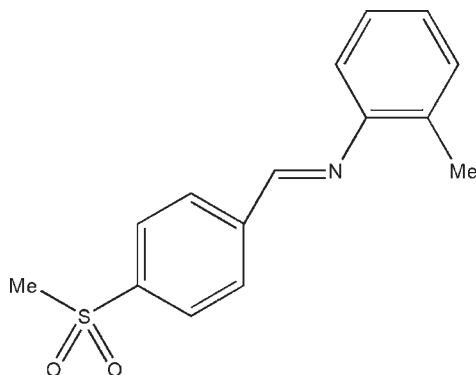
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.044;  $wR$  factor = 0.151; data-to-parameter ratio = 15.1.

Molecules of the title compound,  $\text{C}_{15}\text{H}_{15}\text{NO}_2\text{S}$ , display an *E* configuration with respect to the  $\text{C}=\text{N}$  double bond. The crystal structure is stabilized by weak  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds. The dihedral angle between the two aromatic ring planes is  $50.41$  ( $12$ )°.

### Related literature

For background to Schiff base compounds in coordination chemistry, see: Shao *et al.* (2004).



### Experimental

#### Crystal data

$\text{C}_{15}\text{H}_{15}\text{NO}_2\text{S}$   
 $M_r = 273.34$   
 Monoclinic,  $P2_1/c$   
 $a = 11.445$  (2) Å  
 $b = 7.8770$  (16) Å  
 $c = 16.132$  (3) Å  
 $\beta = 98.65$  (3)°

$V = 1437.8$  (5) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.22$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.30 \times 0.20 \times 0.20$  mm

#### Data collection

Enraf-Nonius CAD-4 diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.936$ ,  $T_{\max} = 0.957$   
 2745 measured reflections

2607 independent reflections  
 1898 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$   
 3 standard reflections every 200 reflections  
 intensity decay: 1%

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.151$   
 $S = 1.00$   
 2607 reflections

173 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.28$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.24$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C4}-\text{H4A}\cdots\text{O1}^i$	0.93	2.55	3.274 (3)	135

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

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CAD-4 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: FJ2256).

### References

- Enraf-Nonius (1989). *CAD-4 Software*. Enraf-Nonius, Delft, The Netherlands.  
 Shao, S.-C., You, Z.-L., Fan, S.-H., Tang, L.-L., Xiong, Z.-D. & Zhu, H.-L. (2004). *Acta Cryst.* **E60**, o2183–o2184.  
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

**supplementary materials**

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## (*E*)-2-Methyl-*N*-[4-(methylsulfonyl)benzylidene]aniline

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### Comment

Schiff base compounds have attracted attention for the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Shao *et al.*, 2004). As an extension of work on the structural characterization of Schiff base compounds, the crystal structure of the title compound (I), Figure 1, is reported here. The molecule displays a *trans*-configuration with respect to the C=N double bond. The crystal structure is stabilized by weak C—H $\cdots$ O hydrogen bonds (Figure 2). The dihedral angle between two aromatic ring planes is 50.41 (12) $^\circ$ .

### Experimental

4-(methylsulfonyl)benzaldehyde (0.184g) and *o*-toluidine (0.107g) were dissolved in acetonitrile (20 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. After keeping the solution in air for 10 d, yellow block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

### Refinement

All the H atoms attached to C atoms were placed in geometrical positions and constrained to ride on their parent atoms with C-H distance in the range 0.93–0.98 Å. They were treated as riding atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

### Figures

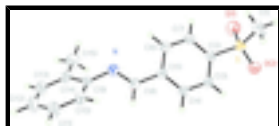


Fig. 1. The structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

## (*E*)-2-Methyl-*N*-[4-(methylsulfonyl)benzylidene]aniline

### Crystal data

$\text{C}_{15}\text{H}_{15}\text{NO}_2\text{S}$

$M_r = 273.34$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2ybc$

$a = 11.445\ (2)\ \text{\AA}$

$b = 7.8770\ (16)\ \text{\AA}$

$c = 16.132\ (3)\ \text{\AA}$

$\beta = 98.65\ (3)^\circ$

$V = 1437.8\ (5)\ \text{\AA}^3$

$F(000) = 576$

$D_x = 1.263\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 25 reflections

$\theta = 9\text{--}14^\circ$

$\mu = 0.22\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Block, yellow

$0.30 \times 0.20 \times 0.20\ \text{mm}$

# supplementary materials

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Z = 4

## Data collection

Enraf–Nonius CAD-4 diffractometer	1898 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\text{int}} = 0.026$
graphite	$\theta_{\text{max}} = 25.3^\circ$ , $\theta_{\text{min}} = 1.8^\circ$
$\omega/2\theta$ scans	$h = 0 \rightarrow 13$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = 0 \rightarrow 9$
$T_{\text{min}} = 0.936$ , $T_{\text{max}} = 0.957$	$l = -19 \rightarrow 19$
2745 measured reflections	3 standard reflections every 200 reflections
2607 independent reflections	intensity decay: 1%

## Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.151$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.09P]$
$S = 1.00$	where $P = (F_o^2 + 2F_c^2)/3$
2607 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
173 parameters	$\Delta\rho_{\text{max}} = 0.28 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.24 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: <i>SHELXTL</i> (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.052 (5)

## Special details

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.43428 (5)	0.25210 (8)	0.34889 (3)	0.0539 (3)
N1	0.01690 (16)	0.3139 (2)	0.60356 (12)	0.0527 (5)

O1	0.35995 (19)	0.2305 (3)	0.27085 (11)	0.0941 (8)
C1	0.5014 (3)	0.4515 (4)	0.3496 (2)	0.1056 (12)
H1B	0.5521	0.4550	0.3074	0.158*
H1C	0.5472	0.4715	0.4036	0.158*
H1D	0.4417	0.5375	0.3383	0.158*
C2	0.3445 (2)	0.2644 (3)	0.42882 (13)	0.0447 (5)
O2	0.52410 (16)	0.1283 (3)	0.37209 (12)	0.0867 (7)
C3	0.38513 (18)	0.1981 (3)	0.50701 (13)	0.0487 (5)
H3A	0.4603	0.1507	0.5183	0.058*
C4	0.31293 (19)	0.2031 (3)	0.56824 (13)	0.0503 (6)
H4A	0.3397	0.1583	0.6210	0.060*
C5	0.20111 (19)	0.2740 (3)	0.55184 (13)	0.0463 (5)
C6	0.1612 (2)	0.3412 (3)	0.47238 (14)	0.0569 (6)
H6A	0.0865	0.3898	0.4610	0.068*
C7	0.2329 (2)	0.3353 (3)	0.41107 (14)	0.0569 (6)
H7A	0.2064	0.3788	0.3580	0.068*
C8	0.12384 (19)	0.2695 (3)	0.61761 (14)	0.0499 (6)
H8A	0.1553	0.2328	0.6711	0.060*
C9	-0.05118 (19)	0.3031 (3)	0.67002 (15)	0.0504 (6)
C10	-0.0096 (2)	0.3600 (3)	0.75031 (16)	0.0617 (6)
H10A	0.0659	0.4057	0.7623	0.074*
C11	-0.0797 (3)	0.3492 (4)	0.81250 (18)	0.0807 (9)
H11A	-0.0511	0.3865	0.8664	0.097*
C12	-0.1918 (3)	0.2837 (4)	0.7949 (2)	0.0881 (10)
H12A	-0.2392	0.2764	0.8367	0.106*
C13	-0.2333 (2)	0.2291 (4)	0.7156 (2)	0.0805 (9)
H13A	-0.3090	0.1833	0.7047	0.097*
C14	-0.1664 (2)	0.2396 (3)	0.65064 (18)	0.0613 (7)
C15	-0.2132 (3)	0.1814 (4)	0.5632 (2)	0.0894 (9)
H15A	-0.2931	0.1428	0.5611	0.134*
H15B	-0.1652	0.0901	0.5478	0.134*
H15C	-0.2111	0.2741	0.5248	0.134*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0647 (4)	0.0564 (4)	0.0429 (4)	0.0082 (3)	0.0156 (3)	0.0032 (2)
N1	0.0492 (11)	0.0500 (11)	0.0603 (12)	0.0039 (9)	0.0122 (9)	0.0041 (9)
O1	0.0922 (14)	0.147 (2)	0.0427 (10)	0.0062 (13)	0.0097 (10)	-0.0103 (11)
C1	0.122 (3)	0.078 (2)	0.135 (3)	-0.0203 (19)	0.078 (2)	-0.001 (2)
C2	0.0524 (12)	0.0402 (11)	0.0421 (11)	0.0007 (9)	0.0093 (9)	0.0013 (9)
O2	0.0940 (13)	0.0980 (16)	0.0764 (12)	0.0453 (12)	0.0395 (11)	0.0257 (11)
C3	0.0436 (11)	0.0587 (13)	0.0426 (11)	0.0065 (10)	0.0019 (9)	-0.0034 (10)
C4	0.0516 (13)	0.0598 (14)	0.0382 (11)	0.0046 (10)	0.0027 (9)	0.0003 (10)
C5	0.0489 (12)	0.0460 (13)	0.0444 (11)	0.0005 (9)	0.0078 (9)	-0.0020 (9)
C6	0.0546 (13)	0.0590 (15)	0.0575 (13)	0.0161 (11)	0.0097 (11)	0.0139 (11)
C7	0.0635 (14)	0.0605 (15)	0.0470 (12)	0.0131 (12)	0.0099 (11)	0.0144 (11)
C8	0.0501 (13)	0.0504 (13)	0.0490 (12)	0.0003 (10)	0.0069 (10)	-0.0014 (10)

## supplementary materials

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C9	0.0466 (12)	0.0421 (11)	0.0642 (14)	0.0031 (9)	0.0140 (10)	0.0026 (10)
C10	0.0569 (13)	0.0595 (15)	0.0708 (15)	0.0010 (12)	0.0159 (11)	-0.0064 (12)
C11	0.087 (2)	0.085 (2)	0.0760 (19)	0.0097 (17)	0.0301 (15)	-0.0102 (15)
C12	0.082 (2)	0.096 (2)	0.098 (2)	0.0081 (18)	0.0495 (19)	0.0055 (19)
C13	0.0546 (16)	0.0719 (19)	0.121 (3)	-0.0029 (13)	0.0317 (17)	0.0098 (18)
C14	0.0500 (13)	0.0496 (14)	0.0848 (18)	0.0007 (11)	0.0124 (12)	0.0043 (12)
C15	0.0661 (17)	0.091 (2)	0.106 (2)	-0.0196 (16)	-0.0010 (16)	-0.0162 (19)

### *Geometric parameters (Å, °)*

S1—O1	1.420 (2)	C6—H6A	0.9300
S1—O2	1.4257 (18)	C7—H7A	0.9300
S1—C1	1.747 (3)	C8—H8A	0.9300
S1—C2	1.768 (2)	C9—C10	1.385 (3)
N1—C8	1.260 (3)	C9—C14	1.401 (3)
N1—C9	1.420 (3)	C10—C11	1.378 (3)
C1—H1B	0.9600	C10—H10A	0.9300
C1—H1C	0.9600	C11—C12	1.372 (4)
C1—H1D	0.9600	C11—H11A	0.9300
C2—C3	1.380 (3)	C12—C13	1.364 (5)
C2—C7	1.384 (3)	C12—H12A	0.9300
C3—C4	1.380 (3)	C13—C14	1.391 (4)
C3—H3A	0.9300	C13—H13A	0.9300
C4—C5	1.385 (3)	C14—C15	1.503 (4)
C4—H4A	0.9300	C15—H15A	0.9600
C5—C6	1.398 (3)	C15—H15B	0.9600
C5—C8	1.480 (3)	C15—H15C	0.9600
C6—C7	1.377 (3)		
O1—S1—O2	117.58 (13)	C6—C7—H7A	120.1
O1—S1—C1	108.53 (17)	C2—C7—H7A	120.1
O2—S1—C1	108.33 (16)	N1—C8—C5	122.2 (2)
O1—S1—C2	108.46 (12)	N1—C8—H8A	118.9
O2—S1—C2	108.73 (10)	C5—C8—H8A	118.9
C1—S1—C2	104.42 (12)	C10—C9—C14	120.2 (2)
C8—N1—C9	118.4 (2)	C10—C9—N1	122.4 (2)
S1—C1—H1B	109.5	C14—C9—N1	117.3 (2)
S1—C1—H1C	109.5	C11—C10—C9	120.3 (2)
H1B—C1—H1C	109.5	C11—C10—H10A	119.8
S1—C1—H1D	109.5	C9—C10—H10A	119.8
H1B—C1—H1D	109.5	C12—C11—C10	120.0 (3)
H1C—C1—H1D	109.5	C12—C11—H11A	120.0
C3—C2—C7	121.0 (2)	C10—C11—H11A	120.0
C3—C2—S1	119.54 (17)	C13—C12—C11	119.7 (3)
C7—C2—S1	119.39 (16)	C13—C12—H12A	120.1
C2—C3—C4	119.2 (2)	C11—C12—H12A	120.1
C2—C3—H3A	120.4	C12—C13—C14	122.2 (3)
C4—C3—H3A	120.4	C12—C13—H13A	118.9
C3—C4—C5	120.7 (2)	C14—C13—H13A	118.9
C3—C4—H4A	119.7	C13—C14—C9	117.4 (3)

C5—C4—H4A	119.7	C13—C14—C15	122.0 (3)
C4—C5—C6	119.5 (2)	C9—C14—C15	120.6 (2)
C4—C5—C8	119.21 (19)	C14—C15—H15A	109.5
C6—C5—C8	121.2 (2)	C14—C15—H15B	109.5
C7—C6—C5	119.9 (2)	H15A—C15—H15B	109.5
C7—C6—H6A	120.1	C14—C15—H15C	109.5
C5—C6—H6A	120.1	H15A—C15—H15C	109.5
C6—C7—C2	119.7 (2)	H15B—C15—H15C	109.5
O1—S1—C2—C3	145.99 (19)	C9—N1—C8—C5	179.03 (19)
O2—S1—C2—C3	17.0 (2)	C4—C5—C8—N1	-171.7 (2)
C1—S1—C2—C3	-98.4 (2)	C6—C5—C8—N1	5.3 (3)
O1—S1—C2—C7	-31.9 (2)	C8—N1—C9—C10	45.4 (3)
O2—S1—C2—C7	-160.84 (19)	C8—N1—C9—C14	-137.8 (2)
C1—S1—C2—C7	83.7 (2)	C14—C9—C10—C11	2.2 (4)
C7—C2—C3—C4	0.0 (3)	N1—C9—C10—C11	179.0 (2)
S1—C2—C3—C4	-177.84 (16)	C9—C10—C11—C12	-0.7 (4)
C2—C3—C4—C5	-0.2 (3)	C10—C11—C12—C13	0.1 (5)
C3—C4—C5—C6	0.0 (3)	C11—C12—C13—C14	-1.0 (5)
C3—C4—C5—C8	177.0 (2)	C12—C13—C14—C9	2.4 (4)
C4—C5—C6—C7	0.5 (4)	C12—C13—C14—C15	-179.1 (3)
C8—C5—C6—C7	-176.5 (2)	C10—C9—C14—C13	-3.0 (3)
C5—C6—C7—C2	-0.7 (4)	N1—C9—C14—C13	-179.9 (2)
C3—C2—C7—C6	0.4 (4)	C10—C9—C14—C15	178.5 (2)
S1—C2—C7—C6	178.29 (19)	N1—C9—C14—C15	1.6 (3)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4A $\cdots$ O1 <sup>i</sup>	0.93	2.55	3.274 (3)	135

Symmetry codes: (i)  $x, -y+1/2, z+1/2$ .

Fig. 1

