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2-Nitrobenzyl methanesulfonate

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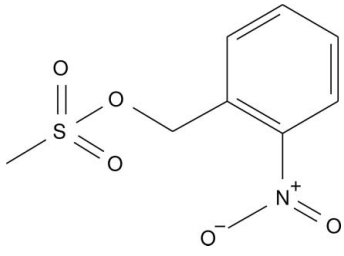
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.112; data-to-parameter ratio = 12.1.

In the title compound, $C_8H_9NO_5S$, the dihedral angle between the benzene ring and the nitro group is 5.86 (15)° and the C—C—O—S group adopts an *anti* conformation [torsion angle = −168.44 (15)°]. In the crystal, molecules are linked by C—H···O hydrogen bonds, generating a three-dimensional network.

Related literature

For background to nitrobenzene derivatives, see: Ranu & Banerjee (2005); Ballini *et al.* (2005). For a related structure, see: Khan *et al.* (2008).



Experimental

Crystal data

$C_8H_9NO_5S$
M_r = 231.23
Monoclinic, $P2_1/c$
a = 12.414 (3) Å
b = 7.967 (2) Å
c = 10.994 (3) Å
β = 112.235 (11)°
V = 1006.5 (5) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.94 mm^{-1}
T = 296 K
0.23 × 0.22 × 0.21 mm

Data collection

Bruker X8 Proteum CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.552, T_{max} = 0.578
6524 measured reflections
1663 independent reflections
1541 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.112
S = 1.08
1663 reflections
138 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.93	2.54	3.266 (3)	135
C3—H3···O2^{ii}	0.93	2.53	3.335 (3)	145
C7—H7*B*···O4^{iii}	0.97	2.58	3.539 (3)	169
C8—H8*A*···O4^{iii}	0.96	2.42	3.374 (4)	172

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, y+1, z$; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*.

We are grateful to the IOE, University of Mysore, for providing the single-crystal X-ray diffraction facility. PN thanks the BET Academy of Higher Education for research facilities.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7217).

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supporting information

Acta Cryst. (2014). E**70**, o616 [doi:10.1107/S160053681400899X]

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S1. Comment

Nitroalkenes have been used as substrates for Michael addition reactions (Ranu & Banerjee, 2005) and for the synthesis of many organic molecules (Ballini *et al.*, 2005).

The *ORTEP* of the title molecule is shown in figure 1. The molecules in the crystal structure are connected with C—H···O hydrogen bonds (Table 1). The C8—H8B···O4 hydrogen bond exhibits ring motifs of the type $R^2_2(8)$. The overall geometry of the title compound is similar to the 3,5-dinitrobenzyl methanesulfonate (Khan *et al.*, 2008). Overall packing of the molecule is shown in figure 2.

S2. Experimental

Red blocks were obtained from slow evaporation of a solution of ethanol.

S3. Refinement

The hydrogen atom were fixed geometrically (C—H= 0.93–0.96 Å) and allowed to ride on their parent atoms with U_{iso}(H) =1.5U_{eq}(*C*-methyl) and = 1.2U_{eq}(C).

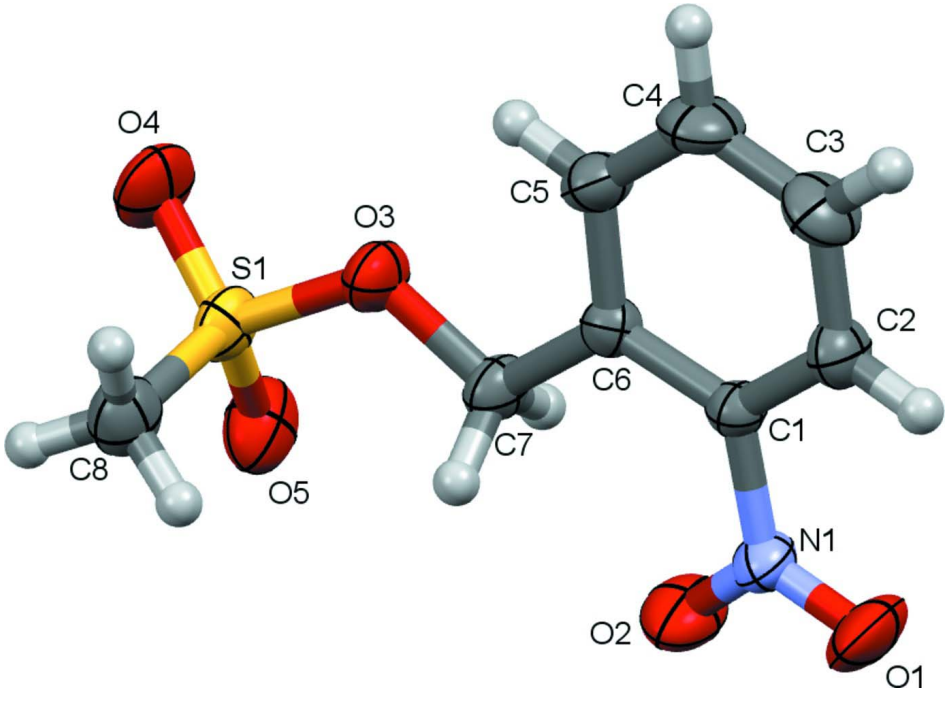

Figure 1

A view of the title molecule, with displacement ellipsoids drawn at the 50% probability level.

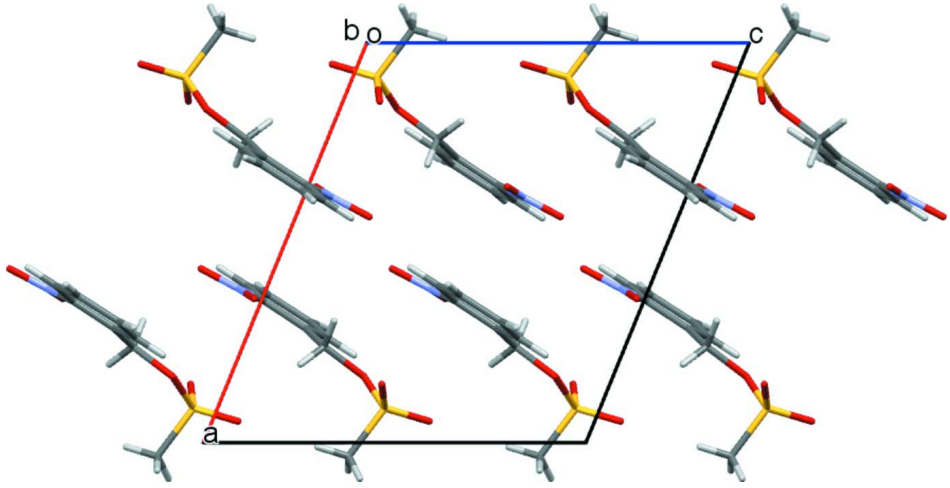

Figure 2

A viewed along the *b* axis of the crystal packing of the title compound.

2-Nitrobenzyl methanesulfonate

Crystal data

$C_8H_9NO_5S$
$M_r = 231.23$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.414$ (3) Å
$b = 7.967$ (2) Å
$c = 10.994$ (3) Å
$\beta = 112.235$ (11)°
$V = 1006.5$ (5) Å^3
$Z = 4$
$F(000) = 480$
$D_x = 1.526$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 1663 reflections
$\theta = 3.8$–$64.5°$
$\mu = 2.94$ mm^{-1}
$T = 296$ K
Block, red
0.23 × 0.22 × 0.21 mm

Data collection

Bruker X8 Proteum CCD diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 10.7 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
$T_{min} = 0.552$, $T_{max} = 0.578$
6524 measured reflections
1663 independent reflections
1541 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 64.5°$, $\theta_{min} = 3.9°$
$h = -14 \rightarrow 13$
$k = -8 \rightarrow 9$
$l = -12 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.112$
$S = 1.08$
1663 reflections
138 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 0.5912P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), FC*=KFC[1+0.001XFC^{2}Λ^3/SIN(2Θ)]$^{-1/4}$
Extinction coefficient: 0.0114 (9)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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}
S1	0.08637 (5)	0.25179 (7)	0.06271 (5)	0.0405 (2)
O1	0.43500 (18)	0.3906 (3)	0.69206 (16)	0.0672 (7)
O2	0.36003 (19)	0.2381 (2)	0.52088 (19)	0.0601 (7)
O3	0.16548 (14)	0.3941 (2)	0.15092 (14)	0.0458 (5)
O4	0.05351 (17)	0.3133 (3)	−0.06740 (15)	0.0592 (7)
O5	0.14617 (16)	0.0958 (2)	0.09607 (18)	0.0584 (6)
N1	0.38559 (15)	0.3744 (2)	0.57357 (17)	0.0376 (6)
C1	0.35397 (16)	0.5255 (2)	0.49184 (19)	0.0295 (6)
C2	0.3940 (2)	0.6755 (3)	0.5560 (2)	0.0411 (7)
C3	0.3686 (2)	0.8231 (3)	0.4862 (3)	0.0523 (9)
C4	0.3040 (2)	0.8185 (3)	0.3534 (3)	0.0533 (9)
C5	0.2634 (2)	0.6678 (3)	0.2901 (2)	0.0424 (7)
C6	0.28708 (17)	0.5157 (3)	0.35717 (19)	0.0310 (6)
C7	0.2405 (2)	0.3532 (3)	0.2870 (2)	0.0387 (7)
C8	−0.0341 (2)	0.2504 (3)	0.1059 (3)	0.0526 (9)
H2	0.43780	0.67660	0.64580	0.0490*
H3	0.39490	0.92490	0.52830	0.0630*
H4	0.28730	0.91790	0.30560	0.0640*
H5	0.21920	0.66820	0.20030	0.0510*
H7A	0.30420	0.28170	0.28830	0.0460*
H7B	0.19630	0.29430	0.32990	0.0460*
H8A	−0.01050	0.22110	0.19700	0.0790*
H8B	−0.08950	0.16960	0.05320	0.0790*
H8C	−0.06920	0.35980	0.09150	0.0790*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0457 (4)	0.0446 (4)	0.0265 (3)	−0.0009 (2)	0.0083 (3)	−0.0091 (2)
O1	0.0821 (13)	0.0607 (13)	0.0332 (10)	0.0016 (10)	−0.0071 (9)	0.0119 (8)
O2	0.0803 (13)	0.0282 (9)	0.0564 (12)	0.0036 (8)	0.0083 (10)	0.0025 (7)

O3	0.0555 (10)	0.0432 (9)	0.0289 (8)	−0.0069 (7)	0.0050 (7)	−0.0037 (7)
O4	0.0670 (11)	0.0806 (14)	0.0262 (9)	−0.0037 (10)	0.0134 (8)	−0.0061 (8)
O5	0.0595 (11)	0.0463 (11)	0.0559 (11)	0.0051 (8)	0.0065 (9)	−0.0161 (8)
N1	0.0376 (9)	0.0337 (10)	0.0345 (10)	0.0023 (7)	0.0056 (8)	0.0053 (8)
C1	0.0322 (10)	0.0256 (10)	0.0298 (10)	0.0008 (8)	0.0106 (8)	0.0013 (8)
C2	0.0463 (12)	0.0365 (12)	0.0349 (12)	−0.0059 (10)	0.0090 (10)	−0.0070 (9)
C3	0.0668 (16)	0.0272 (12)	0.0591 (16)	−0.0085 (11)	0.0197 (13)	−0.0070 (11)
C4	0.0712 (16)	0.0295 (12)	0.0571 (16)	−0.0019 (11)	0.0220 (13)	0.0121 (11)
C5	0.0531 (13)	0.0382 (13)	0.0325 (11)	−0.0006 (10)	0.0123 (10)	0.0058 (9)
C6	0.0339 (10)	0.0299 (11)	0.0303 (10)	−0.0002 (8)	0.0135 (9)	−0.0014 (8)
C7	0.0465 (12)	0.0361 (12)	0.0279 (11)	−0.0004 (9)	0.0079 (9)	−0.0034 (8)
C8	0.0529 (15)	0.0635 (18)	0.0402 (14)	−0.0060 (11)	0.0163 (12)	−0.0060 (11)

Geometric parameters (Å, º)

S1—O3	1.5715 (17)	C4—C5	1.384 (3)
S1—O4	1.4181 (18)	C5—C6	1.391 (3)
S1—O5	1.4227 (18)	C6—C7	1.506 (3)
S1—C8	1.732 (3)	C2—H2	0.9300
O1—N1	1.219 (2)	C3—H3	0.9300
O2—N1	1.215 (2)	C4—H4	0.9300
O3—C7	1.469 (3)	C5—H5	0.9300
N1—C1	1.464 (2)	C7—H7A	0.9700
C1—C2	1.381 (3)	C7—H7B	0.9700
C1—C6	1.399 (3)	C8—H8A	0.9600
C2—C3	1.374 (3)	C8—H8B	0.9600
C3—C4	1.375 (4)	C8—H8C	0.9600
O3—S1—O4	104.31 (11)	O3—C7—C6	107.68 (18)
O3—S1—O5	109.14 (10)	C1—C2—H2	120.00
O3—S1—C8	103.78 (11)	C3—C2—H2	120.00
O4—S1—O5	119.00 (13)	C2—C3—H3	120.00
O4—S1—C8	109.28 (14)	C4—C3—H3	120.00
O5—S1—C8	110.13 (12)	C3—C4—H4	120.00
S1—O3—C7	118.41 (14)	C5—C4—H4	120.00
O1—N1—O2	122.6 (2)	C4—C5—H5	119.00
O1—N1—C1	118.59 (18)	C6—C5—H5	119.00
O2—N1—C1	118.77 (17)	O3—C7—H7A	110.00
N1—C1—C2	115.91 (17)	O3—C7—H7B	110.00
N1—C1—C6	121.17 (17)	C6—C7—H7A	110.00
C2—C1—C6	122.93 (18)	C6—C7—H7B	110.00
C1—C2—C3	119.6 (2)	H7A—C7—H7B	108.00
C2—C3—C4	119.3 (2)	S1—C8—H8A	109.00
C3—C4—C5	120.8 (2)	S1—C8—H8B	110.00
C4—C5—C6	121.7 (2)	S1—C8—H8C	110.00
C1—C6—C5	115.73 (19)	H8A—C8—H8B	109.00
C1—C6—C7	123.31 (19)	H8A—C8—H8C	109.00
C5—C6—C7	120.95 (18)	H8B—C8—H8C	109.00

O4—S1—O3—C7	−163.22 (18)	C2—C1—C6—C5	0.5 (3)
O5—S1—O3—C7	−35.1 (2)	C2—C1—C6—C7	−178.4 (2)
C8—S1—O3—C7	82.36 (19)	N1—C1—C6—C7	1.5 (3)
S1—O3—C7—C6	−168.44 (15)	C1—C2—C3—C4	−0.2 (4)
O1—N1—C1—C2	6.4 (3)	C2—C3—C4—C5	0.8 (4)
O2—N1—C1—C2	−174.7 (2)	C3—C4—C5—C6	−0.7 (4)
O2—N1—C1—C6	5.4 (3)	C4—C5—C6—C1	0.1 (4)
O1—N1—C1—C6	−173.6 (2)	C4—C5—C6—C7	179.0 (2)
C6—C1—C2—C3	−0.4 (4)	C1—C6—C7—O3	174.4 (2)
N1—C1—C6—C5	−179.6 (2)	C5—C6—C7—O3	−4.4 (3)
N1—C1—C2—C3	179.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.93	2.54	3.266 (3)	135
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