

4-Nitrophenyl naphthalene-1-sulfonate

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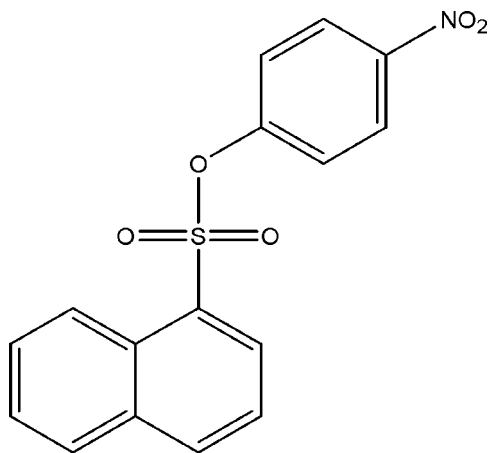
Received 21 August 2008; accepted 25 August 2008

Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.046; wR factor = 0.160; data-to-parameter ratio = 13.5.

In the crystal structure of the title compound, $\text{C}_{16}\text{H}_{11}\text{NO}_5\text{S}$, the plane of the naphthalene ring system forms a dihedral angle of $63.39(8)^\circ$ with the benzene ring. The nitro group makes a dihedral angle of $10.73(16)^\circ$ with the benzene ring. Weak intra- and intermolecular $\text{C}-\text{H}\cdots\text{O}$ interactions are observed.

Related literature

For related literature, see: Manivannan *et al.* (2005); Vennila *et al.* (2008); Yachi *et al.* (1989).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{11}\text{NO}_5\text{S}$

$M_r = 329.32$

Monoclinic, $P2_1/n$

$a = 13.4407(8)$ Å

$b = 6.2990(3)$ Å

$c = 18.2556(12)$ Å

$\beta = 106.296(2)^\circ$

$V = 1483.48(15)$ Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 0.24$ mm⁻¹

$T = 295(2)$ K

$0.28 \times 0.20 \times 0.16$ mm

Data collection

Bruker Kappa APEXII diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.935$, $T_{\max} = 0.962$

14281 measured reflections

2801 independent reflections

1935 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.041$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.160$

$S = 1.08$

2801 reflections

208 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.25$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.20$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C8}-\text{H8}\cdots\text{O2}$	0.93	2.43	2.829 (5)	106
$\text{C16}-\text{H16}\cdots\text{O3}$	0.93	2.46	3.058 (4)	122
$\text{C5}-\text{H5}\cdots\text{O2}^i$	0.93	2.48	3.179 (3)	132
$\text{C15}-\text{H15}\cdots\text{O4}^{ii}$	0.93	2.47	3.340 (5)	155

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

Data collection: APEX2 and SAINT (Bruker, 2004); cell refinement: APEX2; data reduction: APEX2; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

The authors acknowledge the Sophisticated Analytical Instrument Facility, Indian Institute of Technology, Chennai, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2328).

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supplementary materials

Acta Cryst. (2008). E64, o1848 [doi:10.1107/S1600536808027396]

4-Nitrophenyl naphthalene-1-sulfonate

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Comment

The merging of lipids can be monitored using a derivative of *para*-toluene sulfonate (Yachi *et al.*, 1989). The geometric parameters of the title molecule, (I) (Fig. 1), agree well with the reported structures (Manivannan *et al.* 2005; Vennila *et al.* 2008)

The plane of the benzene ring forms a dihedral angle of $63.39(8)^\circ$ with the naphthalene ring system. The torsion angles O2—S1—C7—C8 and O3—S1—C7—C12 [$0.1(3)^\circ$ and $45.8(2)^\circ$, respectively] indicate the *syn* conformation of sulfonyl moiety. The molecular structure is stabilized by weak intramolecular C—H \cdots O interactions and the crystal packing is stabilized by weak intermolecular C—H \cdots O interactions (Fig. 2).

Experimental

1-Naphthalene sulfonyl chloride (2.5 mmol) dissolved in acetone (4 ml) was added dropwise to 4-nitrophenol (2.5 mmol) in aqueous NaOH (4 ml, 5%) with constant shaking. The precipitated compound (1.8 mmol, yield 72%) was recrystallized from ethanol to get diffraction quality pale yellow crystals.

Refinement

H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

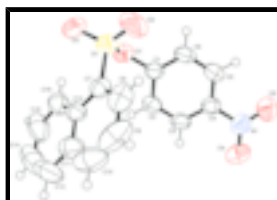


Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

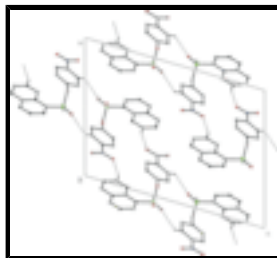


Fig. 2. The packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

4-Nitrophenyl naphthalene-1-sulfonate

Crystal data

$C_{16}H_{11}NO_5S$	$F_{000} = 680$
$M_r = 329.32$	$D_x = 1.474 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
Hall symbol: -P 2yn	$\lambda = 0.71073 \text{ \AA}$
$a = 13.4407 (8) \text{ \AA}$	Cell parameters from 4818 reflections
$b = 6.2990 (3) \text{ \AA}$	$\theta = 2.2\text{--}25.4^\circ$
$c = 18.2556 (12) \text{ \AA}$	$\mu = 0.24 \text{ mm}^{-1}$
$\beta = 106.296 (2)^\circ$	$T = 295 (2) \text{ K}$
$V = 1483.48 (15) \text{ \AA}^3$	Block, yellow
$Z = 4$	$0.28 \times 0.20 \times 0.16 \text{ mm}$

Data collection

Bruker Kappa APEX2 diffractometer	2801 independent reflections
Radiation source: fine-focus sealed tube	1935 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.041$
$T = 295(2) \text{ K}$	$\theta_{\text{max}} = 25.7^\circ$
ω and φ scans	$\theta_{\text{min}} = 1.7^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -16 \rightarrow 16$
$T_{\text{min}} = 0.935$, $T_{\text{max}} = 0.962$	$k = -7 \rightarrow 5$
14281 measured reflections	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	H-atom parameters constrained
$wR(F^2) = 0.160$	$w = 1/[\sigma^2(F_o^2) + (0.0801P)^2 + 0.4092P]$
$S = 1.08$	where $P = (F_o^2 + 2F_c^2)/3$
2801 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
208 parameters	$\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$
	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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S1	0.54713 (6)	0.94373 (13)	0.12153 (4)	0.0704 (3)
C1	0.37278 (18)	0.7401 (4)	0.09748 (13)	0.0528 (6)
C2	0.3303 (2)	0.7033 (4)	0.15655 (14)	0.0598 (6)
H2	0.3391	0.8008	0.1961	0.072*
C3	0.2749 (2)	0.5218 (4)	0.15633 (15)	0.0613 (7)
H3	0.2454	0.4937	0.1957	0.074*
C4	0.26342 (18)	0.3817 (4)	0.09726 (14)	0.0537 (6)
C5	0.3065 (2)	0.4177 (4)	0.03838 (15)	0.0654 (7)
H5	0.2979	0.3198	-0.0010	0.079*
C6	0.3621 (2)	0.5999 (4)	0.03865 (15)	0.0673 (7)
H6	0.3921	0.6277	-0.0005	0.081*
C7	0.58144 (18)	0.8465 (4)	0.21516 (15)	0.0576 (6)
C8	0.6346 (2)	0.6587 (5)	0.2287 (2)	0.0839 (9)
H8	0.6500	0.5851	0.1891	0.101*
C9	0.6658 (3)	0.5785 (7)	0.3043 (4)	0.1117 (16)
H9	0.7032	0.4525	0.3147	0.134*
C10	0.6415 (3)	0.6838 (9)	0.3611 (3)	0.1157 (15)
H10	0.6627	0.6289	0.4103	0.139*
C11	0.5863 (2)	0.8702 (6)	0.34821 (18)	0.0846 (10)
C12	0.55403 (18)	0.9590 (4)	0.27417 (14)	0.0577 (6)
C13	0.5581 (4)	0.9799 (11)	0.4083 (2)	0.1245 (18)
H13	0.5799	0.9270	0.4579	0.149*
C14	0.5005 (4)	1.1579 (11)	0.3943 (3)	0.137 (2)
H14	0.4815	1.2248	0.4337	0.165*
C15	0.4701 (3)	1.2404 (7)	0.3225 (3)	0.1029 (12)
H15	0.4312	1.3647	0.3139	0.124*
C16	0.4949 (2)	1.1465 (5)	0.26351 (18)	0.0725 (8)
H16	0.4725	1.2067	0.2151	0.087*
O1	0.42304 (14)	0.9358 (3)	0.09765 (10)	0.0644 (5)
O2	0.58335 (18)	0.7992 (4)	0.07547 (14)	0.1056 (8)
O3	0.56871 (18)	1.1638 (4)	0.11968 (12)	0.0901 (7)
O4	0.1795 (2)	0.1450 (4)	0.15547 (16)	0.1094 (9)
O5	0.1800 (2)	0.0787 (4)	0.04028 (14)	0.0949 (7)
N1	0.20241 (18)	0.1888 (4)	0.09722 (15)	0.0705 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0768 (5)	0.0848 (6)	0.0604 (5)	-0.0147 (4)	0.0373 (4)	-0.0034 (3)
C1	0.0608 (14)	0.0552 (14)	0.0448 (12)	0.0025 (11)	0.0187 (10)	0.0049 (11)
C2	0.0746 (16)	0.0619 (16)	0.0507 (14)	0.0009 (12)	0.0304 (12)	-0.0052 (12)
C3	0.0741 (16)	0.0690 (17)	0.0507 (15)	0.0013 (13)	0.0337 (12)	0.0051 (12)
C4	0.0581 (14)	0.0527 (14)	0.0511 (14)	0.0055 (11)	0.0168 (11)	0.0068 (11)
C5	0.0781 (17)	0.0737 (18)	0.0491 (14)	-0.0039 (14)	0.0254 (13)	-0.0083 (12)
C6	0.0809 (18)	0.085 (2)	0.0436 (14)	-0.0105 (15)	0.0306 (13)	-0.0030 (13)
C7	0.0517 (13)	0.0586 (15)	0.0676 (16)	-0.0013 (12)	0.0252 (12)	0.0026 (12)
C8	0.0627 (16)	0.0708 (19)	0.124 (3)	0.0023 (15)	0.0362 (18)	-0.0020 (19)
C9	0.065 (2)	0.092 (3)	0.167 (5)	0.0121 (17)	0.014 (2)	0.057 (3)

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C10	0.080 (2)	0.154 (4)	0.098 (3)	-0.011 (3)	0.001 (2)	0.056 (3)
C11	0.0654 (18)	0.120 (3)	0.0612 (19)	-0.0228 (19)	0.0052 (14)	0.0139 (18)
C12	0.0504 (13)	0.0711 (17)	0.0525 (15)	-0.0091 (12)	0.0158 (11)	0.0008 (12)
C13	0.101 (3)	0.224 (6)	0.0479 (19)	-0.057 (3)	0.0186 (19)	-0.009 (3)
C14	0.119 (4)	0.214 (6)	0.096 (4)	-0.058 (4)	0.058 (3)	-0.076 (4)
C15	0.095 (2)	0.116 (3)	0.112 (3)	-0.019 (2)	0.052 (2)	-0.053 (2)
C16	0.0740 (18)	0.0747 (19)	0.0751 (19)	-0.0021 (15)	0.0312 (15)	-0.0112 (15)
O1	0.0746 (12)	0.0641 (12)	0.0561 (11)	-0.0065 (9)	0.0206 (9)	0.0071 (8)
O2	0.1001 (16)	0.145 (2)	0.0946 (16)	-0.0191 (15)	0.0642 (14)	-0.0393 (15)
O3	0.1088 (17)	0.0895 (15)	0.0763 (14)	-0.0348 (12)	0.0328 (12)	0.0139 (11)
O4	0.151 (2)	0.0943 (17)	0.1024 (19)	-0.0314 (15)	0.0678 (18)	0.0109 (14)
O5	0.1127 (19)	0.0819 (16)	0.0837 (17)	-0.0223 (12)	0.0167 (13)	-0.0090 (12)
N1	0.0763 (15)	0.0610 (15)	0.0735 (17)	0.0015 (11)	0.0196 (13)	0.0074 (13)

Geometric parameters (Å, °)

S1—O2	1.415 (2)	C8—C9	1.418 (6)
S1—O3	1.419 (2)	C8—H8	0.9300
S1—O1	1.602 (2)	C9—C10	1.346 (6)
S1—C7	1.751 (3)	C9—H9	0.9300
C1—C6	1.367 (4)	C10—C11	1.374 (6)
C1—C2	1.374 (3)	C10—H10	0.9300
C1—O1	1.405 (3)	C11—C12	1.414 (4)
C2—C3	1.364 (4)	C11—C13	1.435 (6)
C2—H2	0.9300	C12—C16	1.406 (4)
C3—C4	1.368 (4)	C13—C14	1.345 (7)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.375 (4)	C14—C15	1.361 (7)
C4—N1	1.466 (3)	C14—H14	0.9300
C5—C6	1.369 (4)	C15—C16	1.350 (4)
C5—H5	0.9300	C15—H15	0.9300
C6—H6	0.9300	C16—H16	0.9300
C7—C8	1.368 (4)	O4—N1	1.218 (3)
C7—C12	1.422 (4)	O5—N1	1.215 (3)
O2—S1—O3	120.53 (15)	C9—C8—H8	120.6
O2—S1—O1	108.88 (12)	C10—C9—C8	120.3 (4)
O3—S1—O1	103.19 (12)	C10—C9—H9	119.9
O2—S1—C7	108.34 (15)	C8—C9—H9	119.9
O3—S1—C7	111.42 (13)	C9—C10—C11	121.7 (4)
O1—S1—C7	102.92 (10)	C9—C10—H10	119.1
C6—C1—C2	122.2 (2)	C11—C10—H10	119.1
C6—C1—O1	120.9 (2)	C10—C11—C12	120.5 (4)
C2—C1—O1	116.9 (2)	C10—C11—C13	121.8 (4)
C3—C2—C1	119.1 (2)	C12—C11—C13	117.7 (4)
C3—C2—H2	120.5	C16—C12—C11	118.3 (3)
C1—C2—H2	120.5	C16—C12—C7	124.8 (2)
C2—C3—C4	118.9 (2)	C11—C12—C7	116.9 (3)
C2—C3—H3	120.5	C14—C13—C11	121.1 (4)
C4—C3—H3	120.5	C14—C13—H13	119.5

C3—C4—C5	122.1 (2)	C11—C13—H13	119.5
C3—C4—N1	118.3 (2)	C13—C14—C15	120.3 (4)
C5—C4—N1	119.6 (2)	C13—C14—H14	119.9
C6—C5—C4	119.0 (2)	C15—C14—H14	119.9
C6—C5—H5	120.5	C16—C15—C14	121.7 (4)
C4—C5—H5	120.5	C16—C15—H15	119.1
C1—C6—C5	118.8 (2)	C14—C15—H15	119.1
C1—C6—H6	120.6	C15—C16—C12	120.9 (3)
C5—C6—H6	120.6	C15—C16—H16	119.5
C8—C7—C12	121.8 (3)	C12—C16—H16	119.5
C8—C7—S1	117.4 (2)	C1—O1—S1	119.41 (15)
C12—C7—S1	120.8 (2)	O5—N1—O4	123.7 (3)
C7—C8—C9	118.8 (4)	O5—N1—C4	118.6 (2)
C7—C8—H8	120.6	O4—N1—C4	117.7 (3)
C6—C1—C2—C3	-0.5 (4)	C13—C11—C12—C16	-1.2 (4)
O1—C1—C2—C3	175.8 (2)	C10—C11—C12—C7	0.1 (4)
C1—C2—C3—C4	0.1 (4)	C13—C11—C12—C7	-179.1 (3)
C2—C3—C4—C5	0.4 (4)	C8—C7—C12—C16	-176.5 (3)
C2—C3—C4—N1	-179.1 (2)	S1—C7—C12—C16	3.0 (3)
C3—C4—C5—C6	-0.3 (4)	C8—C7—C12—C11	1.3 (4)
N1—C4—C5—C6	179.1 (2)	S1—C7—C12—C11	-179.13 (19)
C2—C1—C6—C5	0.5 (4)	C10—C11—C13—C14	-177.4 (4)
O1—C1—C6—C5	-175.6 (2)	C12—C11—C13—C14	1.8 (6)
C4—C5—C6—C1	-0.1 (4)	C11—C13—C14—C15	-1.7 (7)
O2—S1—C7—C8	0.1 (3)	C13—C14—C15—C16	0.9 (7)
O3—S1—C7—C8	-134.7 (2)	C14—C15—C16—C12	-0.3 (5)
O1—S1—C7—C8	115.3 (2)	C11—C12—C16—C15	0.5 (4)
O2—S1—C7—C12	-179.42 (19)	C7—C12—C16—C15	178.3 (3)
O3—S1—C7—C12	45.8 (2)	C6—C1—O1—S1	-78.7 (3)
O1—S1—C7—C12	-64.2 (2)	C2—C1—O1—S1	104.9 (2)
C12—C7—C8—C9	-2.0 (4)	O2—S1—O1—C1	54.4 (2)
S1—C7—C8—C9	178.4 (2)	O3—S1—O1—C1	-176.40 (18)
C7—C8—C9—C10	1.3 (5)	C7—S1—O1—C1	-60.4 (2)
C8—C9—C10—C11	0.1 (6)	C3—C4—N1—O5	170.0 (3)
C9—C10—C11—C12	-0.8 (5)	C5—C4—N1—O5	-9.4 (4)
C9—C10—C11—C13	178.4 (4)	C3—C4—N1—O4	-12.0 (4)
C10—C11—C12—C16	178.0 (3)	C5—C4—N1—O4	168.5 (3)

Hydrogen-bond geometry (Å, °)

<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>
C8—H8 \cdots O2	0.93	2.43	2.829 (5)	106
C16—H16 \cdots O3	0.93	2.46	3.058 (4)	122
C5—H5 \cdots O2 ⁱ	0.93	2.48	3.179 (3)	132
C15—H15 \cdots O4 ⁱⁱ	0.93	2.47	3.340 (5)	155

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+1/2, y+3/2, -z+1/2$.

Fig. 1

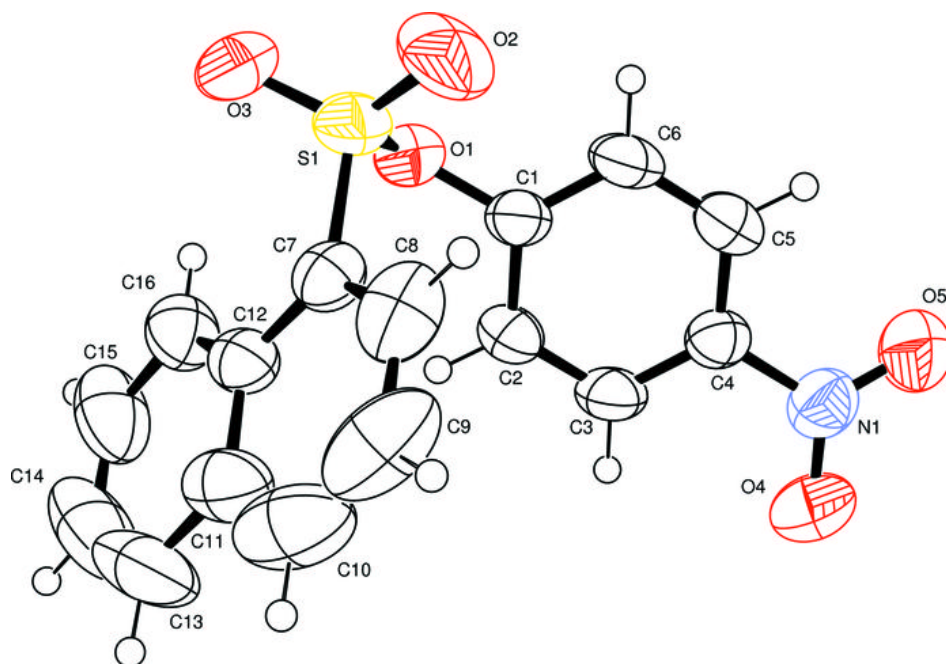


Fig. 2

