

4-Aminophenyl naphthalene-1-sulfonate

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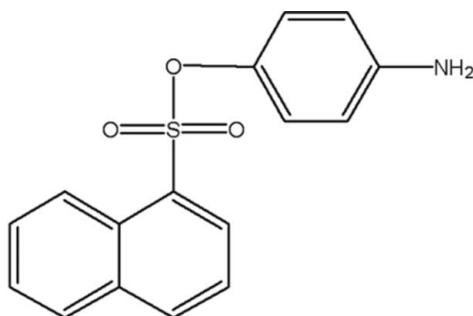
Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å;

R factor = 0.052; wR factor = 0.164; data-to-parameter ratio = 24.4.

In the title compound, $\text{C}_{16}\text{H}_{13}\text{NO}_3\text{S}$, the plane of the aminobenzene ring makes a dihedral angle of $61.04(6)^\circ$ with the naphthalene ring system. Both ring systems form weak intramolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds with the sulfonate group. In the crystal structure, weak intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds and a $\text{C}-\text{H}\cdots\pi$ interaction are observed.

Related literature

For biological activity, see: Yachi *et al.* (1989). For the structures of closely related compounds, see: Manivannan *et al.* (2005a,b).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{13}\text{NO}_3\text{S}$

$M_r = 299.33$

Orthorhombic, $P2_12_12_1$

$a = 7.0456(3)$ Å

$b = 12.4789(6)$ Å

$c = 15.8064(8)$ Å

$V = 1389.72(11)$ Å³

$Z = 4$

Mo $K\alpha$ radiation
 $\mu = 0.24$ mm⁻¹

$T = 295(2)$ K
 $0.36 \times 0.16 \times 0.16$ mm

Data collection

Bruker Kappa APEXII
diffractometer

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.918$, $T_{\max} = 0.962$

19808 measured reflections
4629 independent reflections
3267 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$

$wR(F^2) = 0.164$

$S = 1.03$

4629 reflections

190 parameters

2 restraints

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.44$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.37$ e Å⁻³

Absolute structure: Flack (1983),

1972 Friedel pairs

Flack parameter: $-0.01(10)$

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C6}-\text{H6}\cdots\text{O3}$	0.93	2.52	3.038 (3)	116
$\text{C8}-\text{H8}\cdots\text{O3}$	0.93	2.38	2.804 (4)	108
$\text{C15}-\text{H15}\cdots\text{O2}$	0.93	2.44	3.071 (4)	125
$\text{N1}-\text{H1B}\cdots\text{O1}^{\text{i}}$	0.86	2.05	2.909 (3)	173
$\text{N1}-\text{H1A}\cdots\text{O3}^{\text{ii}}$	0.86	1.94	2.773 (3)	162
$\text{C6}-\text{H6}\cdots\text{Cg}^{\text{iii}}$	0.93	2.84	3.380 (3)	107

Symmetry codes: (i) $-x, y - \frac{1}{2}, -z + \frac{3}{2}$; (ii) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$; (iii) $-x + \frac{1}{2}, -y, z + \frac{1}{2}$. Cg is the centroid of the C11–C16 ring.

Data collection: *APEX2* (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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2293).

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supplementary materials

Acta Cryst. (2008). E64, o1124 [doi:10.1107/S1600536808014438]

4-Aminophenyl naphthalene-1-sulfonate

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Comment

Several compounds containing *para*-toluene sulfonate moiety are used in the fields of biology and industry. The merging of lipids can be monitored using a derivative of *para*-toluene sulfonate (Yachi *et al.*, 1989).

We report the crystal structure of the title compound, (I). The geometric parameters of the molecule of (I) (Fig. 1) agree well with the reported structures (Manivannan *et al.* 2005*a,b*). The plane of the aminobenzene ring forms a dihedral angle of 61.04 (6)° with the naphthalene ring.

The molecular structure is stabilized by weak intramolecular C—H···O interactions and the crystal packing is stabilized by weak intermolecular N—H···O interactions and a C—H··· π interaction (Table 1), involving the ring C11—C16 (centroid *Cg*).

Experimental

1-Naphthalene sulfonyl chloride (5 mmol) dissolved in acetone (4 ml) was added dropwise to *p*-amino phenol (5 mmol) in aqueous NaOH (4 ml, 5%) with constant shaking. The precipitated compound (3.5 mmol, yield 70%) was recrystlized from ethanol.

Refinement

H atoms were positioned geometrically (C—H = 0.93 and N—H = 0.86 Å) and refined using riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$. The anisotropic displacement parameters of O1, S1 and C1 atoms were refined with a rigid bond restraint (DELU) in the final cycles of refinement.

Figures

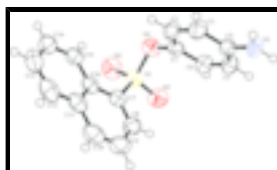


Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms. Intramolecular H-bonds are shown as dotted lines.

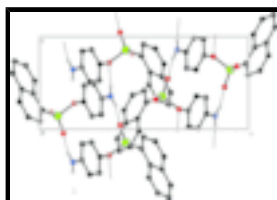


Fig. 2. The packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

4-Aminophenyl naphthalene-1-sulfonate

Crystal data

$C_{16}H_{13}NO_3S$	$F_{000} = 624$
$M_r = 299.33$	$D_x = 1.431 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
Hall symbol: P 2ac 2ab	$\lambda = 0.71073 \text{ \AA}$
$a = 7.0456 (3) \text{ \AA}$	Cell parameters from 4586 reflections
$b = 12.4789 (6) \text{ \AA}$	$\theta = 2.8\text{--}25.7^\circ$
$c = 15.8064 (8) \text{ \AA}$	$\mu = 0.24 \text{ mm}^{-1}$
$V = 1389.72 (11) \text{ \AA}^3$	$T = 295 (2) \text{ K}$
$Z = 4$	Block, brown
	$0.36 \times 0.16 \times 0.16 \text{ mm}$

Data collection

Bruker Kappa APEXII diffractometer	4629 independent reflections
Radiation source: fine-focus sealed tube	3267 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.030$
$T = 295(2) \text{ K}$	$\theta_{\text{max}} = 31.9^\circ$
ω and φ scans	$\theta_{\text{min}} = 2.1^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 10$
$T_{\text{min}} = 0.918$, $T_{\text{max}} = 0.962$	$k = -18 \rightarrow 18$
19808 measured reflections	$l = -23 \rightarrow 19$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.051$	$w = 1/[\sigma^2(F_o^2) + (0.0956P)^2 + 0.1498P]$
$wR(F^2) = 0.164$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} < 0.001$
4629 reflections	$\Delta\rho_{\text{max}} = 0.44 \text{ e \AA}^{-3}$
190 parameters	$\Delta\rho_{\text{min}} = -0.37 \text{ e \AA}^{-3}$
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1972 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: $-0.01 (10)$

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	0.2028 (3)	-0.04132 (18)	0.71108 (14)	0.0415 (4)
C2	0.0284 (3)	-0.0930 (2)	0.71475 (17)	0.0508 (6)
H2	-0.0763	-0.0641	0.6871	0.061*
C3	0.0110 (3)	-0.1874 (2)	0.7597 (2)	0.0545 (6)
H3	-0.1064	-0.2211	0.7637	0.065*
C4	0.1674 (3)	-0.23186 (18)	0.79873 (15)	0.0443 (5)
C5	0.3412 (3)	-0.18155 (19)	0.79520 (16)	0.0488 (5)
H5	0.4463	-0.2117	0.8217	0.059*
C6	0.3577 (3)	-0.08513 (19)	0.75158 (17)	0.0503 (5)
H6	0.4740	-0.0500	0.7497	0.060*
C7	0.2918 (4)	-0.0253 (2)	0.51224 (15)	0.0462 (5)
C8	0.4146 (4)	-0.1082 (2)	0.5015 (2)	0.0569 (6)
H8	0.5286	-0.1097	0.5311	0.068*
C9	0.3689 (6)	-0.1918 (2)	0.4455 (2)	0.0699 (8)
H9	0.4551	-0.2472	0.4370	0.084*
C10	0.2039 (6)	-0.1927 (2)	0.40449 (19)	0.0634 (7)
H10	0.1759	-0.2496	0.3685	0.076*
C11	0.0689 (4)	-0.1083 (2)	0.41450 (18)	0.0539 (6)
C12	-0.1042 (5)	-0.1111 (3)	0.3724 (2)	0.0664 (8)
H12	-0.1329	-0.1691	0.3377	0.080*
C13	-0.2326 (5)	-0.0302 (3)	0.38116 (19)	0.0685 (8)
H13	-0.3481	-0.0328	0.3527	0.082*
C14	-0.1884 (4)	0.0572 (3)	0.43368 (18)	0.0621 (7)
H14	-0.2748	0.1131	0.4393	0.074*
C15	-0.0212 (4)	0.0612 (2)	0.47630 (17)	0.0515 (6)
H15	0.0046	0.1198	0.5108	0.062*
C16	0.1133 (3)	-0.02101 (18)	0.46937 (15)	0.0451 (5)
N1	0.1446 (3)	-0.32773 (15)	0.83938 (13)	0.0487 (5)
H1A	0.2400	-0.3580	0.8635	0.058*
H1B	0.0348	-0.3578	0.8408	0.058*
O1	0.2166 (3)	0.05975 (15)	0.66776 (12)	0.0592 (5)
O2	0.3197 (4)	0.17748 (15)	0.55522 (14)	0.0706 (6)
O3	0.5453 (3)	0.04850 (19)	0.61441 (14)	0.0659 (6)
S1	0.35628 (9)	0.07323 (5)	0.58673 (4)	0.04995 (18)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0433 (10)	0.0422 (9)	0.0391 (11)	-0.0016 (8)	-0.0002 (9)	-0.0121 (8)
C2	0.0377 (10)	0.0564 (14)	0.0584 (15)	-0.0005 (9)	-0.0021 (10)	0.0099 (12)
C3	0.0381 (10)	0.0611 (15)	0.0644 (16)	-0.0067 (10)	-0.0023 (10)	0.0090 (14)
C4	0.0447 (11)	0.0441 (11)	0.0440 (12)	-0.0009 (9)	0.0012 (9)	0.0003 (9)
C5	0.0444 (11)	0.0485 (12)	0.0535 (14)	-0.0027 (10)	-0.0119 (10)	-0.0009 (11)
C6	0.0442 (10)	0.0461 (12)	0.0607 (15)	-0.0082 (10)	-0.0094 (11)	-0.0036 (11)

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C7	0.0534 (12)	0.0399 (11)	0.0452 (12)	-0.0093 (9)	0.0063 (10)	-0.0008 (10)
C8	0.0586 (14)	0.0531 (14)	0.0591 (17)	0.0050 (11)	0.0030 (13)	0.0016 (12)
C9	0.093 (2)	0.0475 (14)	0.0694 (19)	0.0115 (15)	0.0126 (18)	-0.0080 (14)
C10	0.088 (2)	0.0484 (14)	0.0536 (15)	-0.0082 (13)	0.0071 (15)	-0.0097 (13)
C11	0.0719 (15)	0.0475 (13)	0.0423 (13)	-0.0153 (11)	0.0063 (12)	-0.0005 (11)
C12	0.083 (2)	0.0687 (18)	0.0474 (15)	-0.0234 (16)	-0.0050 (14)	-0.0016 (14)
C13	0.0637 (17)	0.092 (2)	0.0500 (15)	-0.0171 (16)	-0.0091 (13)	0.0141 (17)
C14	0.0585 (14)	0.0730 (19)	0.0547 (15)	0.0032 (13)	0.0028 (12)	0.0103 (14)
C15	0.0569 (13)	0.0520 (14)	0.0456 (13)	-0.0040 (10)	0.0064 (10)	0.0026 (11)
C16	0.0550 (12)	0.0409 (11)	0.0395 (11)	-0.0095 (9)	0.0054 (10)	0.0018 (9)
N1	0.0379 (8)	0.0452 (10)	0.0631 (13)	-0.0036 (8)	-0.0047 (9)	0.0182 (9)
O1	0.0663 (10)	0.0520 (9)	0.0594 (10)	-0.0055 (8)	0.0036 (8)	-0.0032 (8)
O2	0.0897 (16)	0.0419 (10)	0.0803 (14)	-0.0233 (10)	0.0025 (12)	0.0052 (10)
O3	0.0465 (9)	0.0750 (14)	0.0763 (13)	-0.0157 (9)	0.0011 (9)	-0.0054 (11)
S1	0.0510 (3)	0.0416 (3)	0.0573 (4)	-0.0135 (2)	0.0011 (3)	-0.0021 (3)

Geometric parameters (Å, °)

C1—C6	1.378 (3)	C9—H9	0.9300
C1—C2	1.389 (3)	C10—C11	1.428 (5)
C1—O1	1.438 (3)	C10—H10	0.9300
C2—C3	1.381 (4)	C11—C12	1.390 (4)
C2—H2	0.9300	C11—C16	1.427 (3)
C3—C4	1.380 (3)	C12—C13	1.362 (5)
C3—H3	0.9300	C12—H12	0.9300
C4—N1	1.368 (3)	C13—C14	1.406 (5)
C4—C5	1.377 (3)	C13—H13	0.9300
C5—C6	1.392 (3)	C14—C15	1.358 (4)
C5—H5	0.9300	C14—H14	0.9300
C6—H6	0.9300	C15—C16	1.401 (4)
C7—C8	1.360 (4)	C15—H15	0.9300
C7—C16	1.430 (3)	N1—H1A	0.8600
C7—S1	1.762 (3)	N1—H1B	0.8600
C8—C9	1.404 (4)	O2—S1	1.417 (2)
C8—H8	0.9300	O3—S1	1.436 (2)
C9—C10	1.332 (5)	O1—S1	1.624 (2)
C6—C1—C2	119.8 (2)	C11—C10—H10	119.3
C6—C1—O1	121.0 (2)	C12—C11—C16	120.2 (3)
C2—C1—O1	119.1 (2)	C12—C11—C10	120.8 (3)
C3—C2—C1	119.7 (2)	C16—C11—C10	119.0 (3)
C3—C2—H2	120.1	C13—C12—C11	121.0 (3)
C1—C2—H2	120.1	C13—C12—H12	119.5
C4—C3—C2	120.1 (2)	C11—C12—H12	119.5
C4—C3—H3	119.9	C12—C13—C14	119.2 (3)
C2—C3—H3	119.9	C12—C13—H13	120.4
N1—C4—C5	121.5 (2)	C14—C13—H13	120.4
N1—C4—C3	117.9 (2)	C15—C14—C13	120.9 (3)
C5—C4—C3	120.6 (2)	C15—C14—H14	119.5
C4—C5—C6	119.2 (2)	C13—C14—H14	119.5

C4—C5—H5	120.4	C14—C15—C16	121.4 (3)
C6—C5—H5	120.4	C14—C15—H15	119.3
C1—C6—C5	120.5 (2)	C16—C15—H15	119.3
C1—C6—H6	119.8	C15—C16—C11	117.3 (2)
C5—C6—H6	119.8	C15—C16—C7	125.8 (2)
C8—C7—C16	121.9 (2)	C11—C16—C7	116.9 (2)
C8—C7—S1	116.8 (2)	C4—N1—H1A	120.0
C16—C7—S1	121.19 (19)	C4—N1—H1B	120.0
C7—C8—C9	119.9 (3)	H1A—N1—H1B	120.0
C7—C8—H8	120.1	C1—O1—S1	120.50 (15)
C9—C8—H8	120.1	O2—S1—O3	118.25 (13)
C10—C9—C8	120.9 (3)	O2—S1—O1	105.20 (13)
C10—C9—H9	119.6	O3—S1—O1	107.43 (12)
C8—C9—H9	119.6	O2—S1—C7	111.02 (13)
C9—C10—C11	121.4 (3)	O3—S1—C7	107.04 (13)
C9—C10—H10	119.3	O1—S1—C7	107.38 (11)
C6—C1—C2—C3	0.7 (4)	C14—C15—C16—C11	1.1 (4)
O1—C1—C2—C3	-176.8 (2)	C14—C15—C16—C7	-179.1 (2)
C1—C2—C3—C4	-1.9 (4)	C12—C11—C16—C15	-1.9 (4)
C2—C3—C4—N1	-177.2 (2)	C10—C11—C16—C15	178.9 (2)
C2—C3—C4—C5	1.6 (4)	C12—C11—C16—C7	178.3 (2)
N1—C4—C5—C6	178.7 (2)	C10—C11—C16—C7	-1.0 (3)
C3—C4—C5—C6	-0.1 (4)	C8—C7—C16—C15	-179.7 (3)
C2—C1—C6—C5	0.9 (4)	S1—C7—C16—C15	4.3 (3)
O1—C1—C6—C5	178.3 (2)	C8—C7—C16—C11	0.1 (3)
C4—C5—C6—C1	-1.1 (4)	S1—C7—C16—C11	-175.90 (18)
C16—C7—C8—C9	1.4 (4)	C6—C1—O1—S1	63.1 (3)
S1—C7—C8—C9	177.6 (2)	C2—C1—O1—S1	-119.4 (2)
C7—C8—C9—C10	-2.0 (5)	C1—O1—S1—O2	174.10 (17)
C8—C9—C10—C11	1.2 (5)	C1—O1—S1—O3	-59.1 (2)
C9—C10—C11—C12	-178.9 (3)	C1—O1—S1—C7	55.8 (2)
C9—C10—C11—C16	0.4 (4)	C8—C7—S1—O2	137.0 (2)
C16—C11—C12—C13	1.4 (4)	C16—C7—S1—O2	-46.8 (2)
C10—C11—C12—C13	-179.4 (3)	C8—C7—S1—O3	6.6 (2)
C11—C12—C13—C14	0.0 (4)	C16—C7—S1—O3	-177.21 (18)
C12—C13—C14—C15	-0.8 (4)	C8—C7—S1—O1	-108.5 (2)
C13—C14—C15—C16	0.3 (4)	C16—C7—S1—O1	67.7 (2)

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>
C6—H6 \cdots O3	0.93	2.52	3.038 (3)	116
C8—H8 \cdots O3	0.93	2.38	2.804 (4)	108
C15—H15 \cdots O2	0.93	2.44	3.071 (4)	125
N1—H1B \cdots O1 ⁱ	0.86	2.05	2.909 (3)	173
N1—H1A \cdots O3 ⁱⁱ	0.86	1.94	2.773 (3)	162
C6—H6 \cdots Cg ⁱⁱⁱ	0.93	2.84	3.380 (3)	107

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

Fig. 1

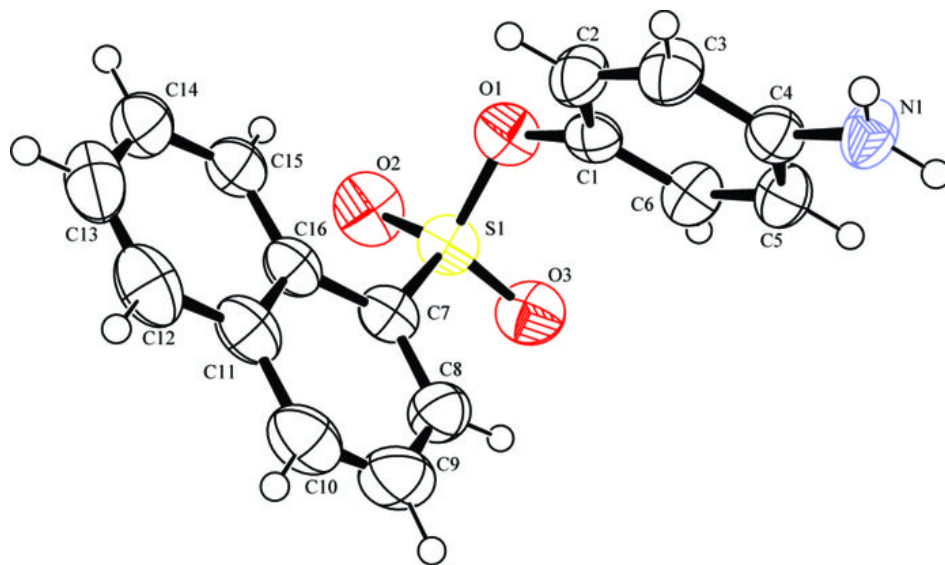


Fig. 2

