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N-(4-Methoxybenzyl)quinoline-8-sulfonamide

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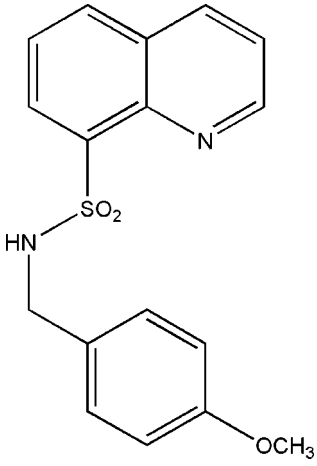
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.004 Å; R factor = 0.044; wR factor = 0.120; data-to-parameter ratio = 13.0.

In the title compound, $C_{17}H_{16}N_2O_3S$, the dihedral angle between the planes of the nearly planar quinoline group and the benzene group of the methoxybenzene group is 11.92 (9)°. The C—S—N—C torsion angle is 68.6 (2)°. Both sulfonyl O atoms are involved in weak intermolecular hydrogen bonds of types N—H···O (H···O = 2.41 Å) and C—H···O (H···O = 2.52 Å).

Related literature

For related literature, see: Andrighetti-Fröhner *et al.* (2003, 2006); da Silva *et al.* (2006, 2007).



Experimental

Crystal data

$C_{17}H_{16}N_2O_3S$
M_r = 328.38
Orthorhombic, $P2_12_12_1$
a = 7.273 (1) Å
b = 9.146 (1) Å
c = 22.975 (3) Å
V = 1528.3 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.03 mm^{-1}
T = 299 (2) K
0.65 × 0.40 × 0.35 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
3007 measured reflections
2724 independent reflections
2684 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.120
S = 1.11
2724 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: (Flack, 1983), 1125 Friedel pairs
Flack parameter: 0.02 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O2^{i}	0.86	2.41	3.094 (3)	137
C6—H6···O1^{ii}	0.93	2.52	3.420 (4)	162

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{5}{2}, -z$; (ii) $x, y-1, z$.

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC Software*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); 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: BH2105).

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supplementary materials

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N-(4-Methoxybenzyl)quinoline-8-sulfonamide

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Comment

The quinoline core is present in many different biological active compounds. We have pursed a pharmacological program to investigate the structure-function relationships, in order to develop antiparasitic and antiviral drugs based on heterocyclic compounds (Andrighetti-Fröhner *et al.*, 2006; da Silva *et al.*, 2007). Our interest in biological active compounds, as potential agents for antiviral diseases (Andrighetti-Fröhner *et al.*, 2003) led to the X-ray study of the title compound, (I).

In the molecule of (I) (Fig. 1) the torsion angle C10—N1—S1—C1 is 68.6 (2)° and the quinoline ring system plane, C1···C9/N2 forms a dihedral angle of 11.92 (9)° with the plane of the benzene group of the methoxybenzene moiety, C11···C16. The quinoline moiety is nearly planar with maximum deviations from the mean plane of −0.0340 (3) Å for atom C7 and 0.0296 (2) Å for atom N2. Two weak intermolecular hydrogen bonds of types N—H···O and C—H···O are observed, which connect molecules to form a three dimensional network (Fig. 2).

Experimental

The title compound was prepared according to the literature procedure (da Silva *et al.*, 2006). Single crystals suitable for X-ray data collection were obtained by recrystallization from a methanol-dichloromethane solution (1:1).

Refinement

H atoms were positioned with idealized geometry and refined using a riding model with C—H and N—H bond lengths constrained to 0.93–0.97 and 0.86 Å, respectively. Their isotropic displacement parameters were set equal to $1.2U_{eq}$ (parent atom).

Figures

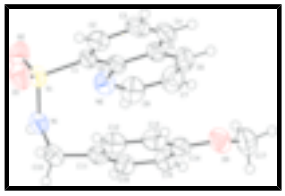

Fig. 1. Molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.

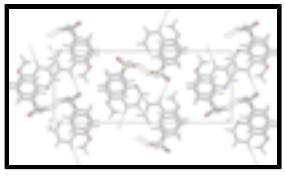

Fig. 2. Molecular packing of (I) with hydrogen bonds shown as dashed lines.

N-(4-Methoxybenzyl)quinoline-8-sulfonamide

Crystal data

$C_{17}H_{16}N_2O_3S$	F_{000} = 688
M_r = 328.38	D_x = 1.427 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Cu $K\alpha$ radiation λ = 1.54180 Å
Hall symbol: P 2ac 2ab	Cell parameters from 25 reflections
a = 7.273 (1) Å	θ = 6.4–18.8º
b = 9.146 (1) Å	μ = 2.03 mm^{-1}
c = 22.975 (3) Å	T = 299 (2) K
V = 1528.3 (3) Å^3	Prism, colourless
Z = 4	0.65 × 0.40 × 0.35 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.075
Radiation source: fine-focus sealed tube	θ_{max} = 67.0º
Monochromator: graphite	θ_{min} = 3.9º
T = 299(2) K	h = 0→8
ω/2θ scans	k = −10→10
Absorption correction: none	l = −27→0
3007 measured reflections	3 standard reflections
2724 independent reflections	every 120 min
2684 reflections with $I > 2\sigma(I)$	intensity decay: 1.0%

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.08P)^2 + 0.3281P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$(\Delta/\sigma)_{max}$ = 0.005
$wR(F^2)$ = 0.120	$\Delta\rho_{max}$ = 0.37 e Å^{-3}
S = 1.11	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
2724 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
210 parameters	Extinction coefficient: 0.0078 (8)
Primary atom site location: structure-invariant direct methods	Absolute structure: (Flack, 1983), 1125 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.02 (2)
Hydrogen site location: inferred from neighbouring sites	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.34694 (9)	1.29117 (6)	0.09586 (3)	0.0453 (2)
O1	0.3555 (3)	1.3926 (2)	0.14329 (9)	0.0636 (5)
O2	0.4836 (3)	1.2999 (2)	0.05121 (9)	0.0628 (5)
O3	−0.1936 (3)	0.7783 (2)	0.20022 (8)	0.0627 (5)
N1	0.1504 (3)	1.3143 (2)	0.06407 (9)	0.0488 (5)
H1N	0.1455	1.3204	0.0267	0.059*
N2	0.2562 (3)	1.0071 (3)	0.03640 (9)	0.0502 (5)
C1	0.3545 (3)	1.1131 (3)	0.12712 (10)	0.0410 (5)
C2	0.4028 (4)	1.1002 (3)	0.18424 (11)	0.0487 (6)
H2	0.4329	1.1831	0.2057	0.058*
C3	0.4070 (4)	0.9610 (4)	0.21093 (13)	0.0572 (7)
H3	0.4444	0.9521	0.2495	0.069*
C4	0.3568 (4)	0.8407 (3)	0.18066 (13)	0.0566 (7)
H4	0.3566	0.7501	0.1990	0.068*
C5	0.3044 (4)	0.8507 (3)	0.12124 (12)	0.0490 (6)
C6	0.2484 (4)	0.7293 (3)	0.08807 (15)	0.0636 (8)
H6	0.2483	0.6363	0.1045	0.076*
C7	0.1941 (5)	0.7485 (4)	0.03161 (16)	0.0699 (9)
H7	0.1531	0.6699	0.0094	0.084*
C8	0.2017 (5)	0.8899 (4)	0.00795 (13)	0.0621 (8)
H8	0.1656	0.9016	−0.0306	0.074*
C9	0.3061 (3)	0.9891 (3)	0.09362 (11)	0.0420 (5)
C10	−0.0218 (4)	1.3251 (3)	0.09868 (14)	0.0567 (7)
H10A	−0.1188	1.3620	0.0737	0.068*
H10B	−0.0033	1.3957	0.1296	0.068*
C11	−0.0842 (3)	1.1829 (3)	0.12522 (11)	0.0460 (6)
C12	−0.0715 (4)	1.1593 (3)	0.18508 (12)	0.0542 (7)
H12	−0.0348	1.2352	0.2094	0.065*
C13	−0.1128 (4)	1.0248 (3)	0.20857 (12)	0.0560 (7)
H13	−0.1052	1.0111	0.2486	0.067*
C14	−0.1650 (4)	0.9106 (3)	0.17343 (10)	0.0456 (5)
C15	−0.1858 (4)	0.9332 (3)	0.11396 (10)	0.0462 (5)
H15	−0.2258	0.8578	0.0900	0.055*
C16	−0.1462 (4)	1.0699 (3)	0.09090 (10)	0.0465 (5)
H16	−0.1619	1.0855	0.0512	0.056*
C17	−0.2180 (5)	0.6546 (4)	0.16410 (16)	0.0717 (9)
H17A	−0.3369	0.6589	0.1460	0.086*
H17B	−0.2091	0.5673	0.1871	0.086*
H17C	−0.1245	0.6535	0.1346	0.086*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0539 (4)	0.0362 (3)	0.0458 (3)	−0.0037 (3)	−0.0012 (3)	0.0070 (2)

O1	0.0878 (15)	0.0416 (10)	0.0613 (11)	−0.0064 (11)	−0.0133 (11)	−0.0026 (8)
O2	0.0623 (11)	0.0649 (12)	0.0612 (11)	−0.0104 (10)	0.0108 (9)	0.0205 (10)
O3	0.0722 (13)	0.0613 (11)	0.0545 (10)	0.0062 (10)	0.0053 (9)	0.0184 (9)
N1	0.0593 (12)	0.0399 (10)	0.0471 (10)	0.0027 (10)	−0.0036 (10)	0.0098 (8)
N2	0.0598 (13)	0.0480 (12)	0.0426 (10)	0.0022 (10)	0.0044 (9)	0.0007 (9)
C1	0.0408 (11)	0.0381 (11)	0.0440 (11)	0.0049 (10)	0.0022 (10)	0.0096 (9)
C2	0.0471 (13)	0.0534 (15)	0.0457 (13)	0.0060 (11)	−0.0006 (10)	0.0025 (12)
C3	0.0506 (15)	0.0715 (19)	0.0495 (14)	0.0168 (13)	0.0037 (11)	0.0238 (14)
C4	0.0497 (14)	0.0528 (14)	0.0672 (16)	0.0138 (12)	0.0106 (13)	0.0261 (13)
C5	0.0430 (12)	0.0403 (12)	0.0637 (15)	0.0098 (10)	0.0120 (11)	0.0102 (11)
C6	0.0596 (15)	0.0393 (14)	0.092 (2)	0.0055 (12)	0.0213 (16)	0.0064 (14)
C7	0.076 (2)	0.0494 (16)	0.084 (2)	−0.0050 (14)	0.0171 (17)	−0.0196 (15)
C8	0.076 (2)	0.0584 (17)	0.0515 (14)	−0.0013 (15)	0.0080 (13)	−0.0115 (13)
C9	0.0396 (11)	0.0395 (11)	0.0469 (12)	0.0075 (9)	0.0065 (9)	0.0055 (10)
C10	0.0557 (14)	0.0413 (13)	0.0730 (18)	0.0112 (12)	−0.0013 (14)	0.0025 (13)
C11	0.0411 (11)	0.0440 (14)	0.0529 (13)	0.0090 (10)	0.0003 (10)	−0.0015 (11)
C12	0.0536 (14)	0.0598 (16)	0.0492 (13)	0.0054 (12)	−0.0021 (12)	−0.0154 (12)
C13	0.0561 (15)	0.0736 (18)	0.0385 (12)	0.0050 (13)	−0.0034 (11)	0.0015 (13)
C14	0.0420 (12)	0.0523 (13)	0.0427 (12)	0.0074 (11)	0.0026 (10)	0.0076 (10)
C15	0.0503 (13)	0.0480 (13)	0.0401 (11)	0.0000 (11)	−0.0020 (10)	−0.0010 (10)
C16	0.0511 (13)	0.0517 (13)	0.0367 (11)	0.0036 (11)	−0.0034 (11)	0.0047 (10)
C17	0.083 (2)	0.0505 (16)	0.081 (2)	0.0083 (15)	0.0259 (18)	0.0121 (15)

Geometric parameters (Å, °)

S1—O2	1.431 (2)	C6—H6	0.9300
S1—O1	1.433 (2)	C7—C8	1.403 (5)
S1—N1	1.619 (2)	C7—H7	0.9300
S1—C1	1.781 (2)	C8—H8	0.9300
O3—C14	1.373 (3)	C10—C11	1.506 (4)
O3—C17	1.415 (4)	C10—H10A	0.9700
N1—C10	1.486 (4)	C10—H10B	0.9700
N1—H1N	0.8600	C11—C16	1.376 (4)
N2—C8	1.317 (4)	C11—C12	1.395 (4)
N2—C9	1.374 (3)	C12—C13	1.377 (4)
C1—C2	1.364 (3)	C12—H12	0.9300
C1—C9	1.415 (3)	C13—C14	1.374 (4)
C2—C3	1.414 (4)	C13—H13	0.9300
C2—H2	0.9300	C14—C15	1.390 (3)
C3—C4	1.352 (5)	C15—C16	1.388 (4)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.420 (4)	C16—H16	0.9300
C4—H4	0.9300	C17—H17A	0.9600
C5—C6	1.407 (4)	C17—H17B	0.9600
C5—C9	1.416 (3)	C17—H17C	0.9600
C6—C7	1.367 (5)		
O2—S1—O1	118.60 (14)	C7—C8—H8	117.6
O2—S1—N1	106.43 (12)	N2—C9—C1	119.3 (2)
O1—S1—N1	107.28 (13)	N2—C9—C5	122.3 (2)

O2—S1—C1	108.61 (12)	C1—C9—C5	118.3 (2)
O1—S1—C1	106.51 (11)	N1—C10—C11	114.4 (2)
N1—S1—C1	109.18 (11)	N1—C10—H10A	108.7
C14—O3—C17	117.4 (2)	C11—C10—H10A	108.7
C10—N1—S1	120.73 (18)	N1—C10—H10B	108.7
C10—N1—H1N	119.6	C11—C10—H10B	108.7
S1—N1—H1N	119.6	H10A—C10—H10B	107.6
C8—N2—C9	117.2 (2)	C16—C11—C12	118.0 (2)
C2—C1—C9	121.2 (2)	C16—C11—C10	121.0 (2)
C2—C1—S1	118.4 (2)	C12—C11—C10	120.8 (3)
C9—C1—S1	120.40 (17)	C13—C12—C11	120.7 (3)
C1—C2—C3	120.1 (3)	C13—C12—H12	119.7
C1—C2—H2	120.0	C11—C12—H12	119.7
C3—C2—H2	120.0	C14—C13—C12	120.6 (2)
C4—C3—C2	120.3 (2)	C14—C13—H13	119.7
C4—C3—H3	119.9	C12—C13—H13	119.7
C2—C3—H3	119.9	O3—C14—C13	116.6 (2)
C3—C4—C5	121.0 (2)	O3—C14—C15	123.7 (2)
C3—C4—H4	119.5	C13—C14—C15	119.6 (2)
C5—C4—H4	119.5	C16—C15—C14	119.1 (2)
C6—C5—C9	117.7 (3)	C16—C15—H15	120.4
C6—C5—C4	123.2 (3)	C14—C15—H15	120.4
C9—C5—C4	119.1 (3)	C11—C16—C15	121.7 (2)
C7—C6—C5	119.7 (3)	C11—C16—H16	119.1
C7—C6—H6	120.1	C15—C16—H16	119.1
C5—C6—H6	120.1	O3—C17—H17A	109.5
C6—C7—C8	118.3 (3)	O3—C17—H17B	109.5
C6—C7—H7	120.8	H17A—C17—H17B	109.5
C8—C7—H7	120.8	O3—C17—H17C	109.5
N2—C8—C7	124.7 (3)	H17A—C17—H17C	109.5
N2—C8—H8	117.6	H17B—C17—H17C	109.5
O2—S1—N1—C10	−174.4 (2)	S1—C1—C9—N2	1.1 (3)
O1—S1—N1—C10	−46.5 (2)	C2—C1—C9—C5	1.5 (3)
C1—S1—N1—C10	68.6 (2)	S1—C1—C9—C5	−176.59 (18)
O2—S1—C1—C2	115.9 (2)	C6—C5—C9—N2	−0.3 (3)
O1—S1—C1—C2	−12.9 (2)	C4—C5—C9—N2	−179.7 (2)
N1—S1—C1—C2	−128.4 (2)	C6—C5—C9—C1	177.3 (2)
O2—S1—C1—C9	−65.9 (2)	C4—C5—C9—C1	−2.0 (3)
O1—S1—C1—C9	165.3 (2)	S1—N1—C10—C11	−72.1 (3)
N1—S1—C1—C9	49.7 (2)	N1—C10—C11—C16	−67.9 (3)
C9—C1—C2—C3	0.7 (4)	N1—C10—C11—C12	108.6 (3)
S1—C1—C2—C3	178.81 (19)	C16—C11—C12—C13	2.6 (4)
C1—C2—C3—C4	−2.4 (4)	C10—C11—C12—C13	−174.0 (3)
C2—C3—C4—C5	1.9 (4)	C11—C12—C13—C14	0.8 (4)
C3—C4—C5—C6	−179.0 (3)	C17—O3—C14—C13	−170.0 (3)
C3—C4—C5—C9	0.3 (4)	C17—O3—C14—C15	10.0 (4)
C9—C5—C6—C7	−1.5 (4)	C12—C13—C14—O3	176.5 (2)
C4—C5—C6—C7	177.8 (3)	C12—C13—C14—C15	−3.5 (4)
C5—C6—C7—C8	2.0 (5)	O3—C14—C15—C16	−177.4 (2)

C9—N2—C8—C7	−1.2 (5)	C13—C14—C15—C16	2.6 (4)
C6—C7—C8—N2	−0.6 (5)	C12—C11—C16—C15	−3.5 (4)
C8—N2—C9—C1	−176.0 (3)	C10—C11—C16—C15	173.1 (2)
C8—N2—C9—C5	1.6 (4)	C14—C15—C16—C11	1.0 (4)
C2—C1—C9—N2	179.3 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O2^{i}	0.86	2.41	3.094 (3)	137
C6—H6···O1^{ii}	0.93	2.52	3.420 (4)	162

Symmetry codes: (i) *x*−1/2, −*y*+5/2, −*z*; (ii) *x*, *y*−1, *z*.

Fig. 1

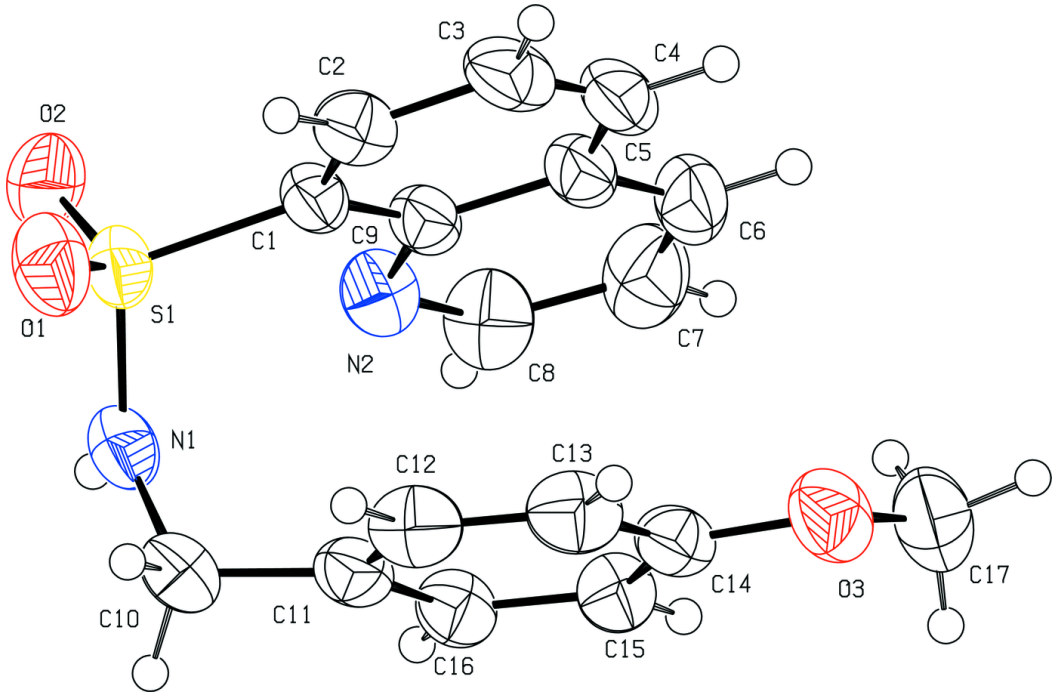
C3
C4
C2
O2
C5
C6
C1
C9
O1
S1
N2
C8
C7
N1
C12
C13
C14
O3
C17
C10
C11
C16
C15

Fig. 2