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2-(2-Furylmethylaminomethyl)-4-sulfanylphenol

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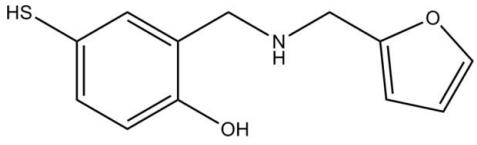
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.058; wR factor = 0.166; data-to-parameter ratio = 14.8.

In the title compound, $C_{12}H_{13}NO_2S$, the dihedral angle between the furan and benzene rings is 62.2 (2)° and an intramolecular O—H···N hydrogen bond is formed. In the crystal, molecules are linked by weak intermolecular N—H···S hydrogen bonds.

Related literature

For background, see: Shi *et al.* (2007). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{12}H_{13}NO_2S$
M_r = 235.29
Orthorhombic, $P2_12_12_1$
a = 5.5778 (12) Å
b = 13.589 (3) Å
c = 14.943 (3) Å
V = 1132.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 293 K
0.30 × 0.30 × 0.10 mm

Data collection

Enraf–Nonius CAD4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.924, T_{max} = 0.974
2528 measured reflections
2216 independent reflections
1811 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
3 standard reflections
every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.166
S = 1.06
2216 reflections
150 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}
Absolute structure: Flack (1983), 900 Friedel pairs
Flack parameter: 0.00 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···N1	0.82	2.04	2.692 (5)	136
N1—H1C···S1^{i}	0.93 (5)	2.90 (4)	3.605 (3)	134 (3)

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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: HB5047).

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supporting information

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2-(2-Furylmethylaminomethyl)-4-sulfanylphenol

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S1. Comment

There has been much research interest in Schiff base compounds due to their biological activities (Shi *et al.*, 2007). In this work, we report here the crystal structure of the title compound, (I). In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). There are an intramolecular O-H···N hydrogen bond and an intermolecular N-H···S hydrogen bond in (I).

S2. Experimental

A mixture of 2-hydroxy-5-mercaptobenzaldehyde (154 mg, 1 mmol) and furan-2-ylmethanamine (97 mg, 1 mmol) were stirred in methanol (10 ml) for 2 h. Then $NaBH_4$ (76 mg, 2 mmol) was added to the reaction solution slowly, and stirred at room temperature for 2 h. The mixture was evaporated under vacuum, and dissolved in dichloromethane (5 ml). The solution was washed with saturated NaCl solution and water, respectively, dried over anhydrous sodium sulfate, and evaporated. Purification by silica gel afforded pure product. Colourless blocks of (I) were obtained by recrystallization of the pure product in methanol.

S3. Refinement

The N-bound H atom was located in a difference map and its position was freely refined. The other H atoms were positioned geometrically (C—H = 0.93–0.97Å, O—H = 0.82Å, S—H = 1.20Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl C).

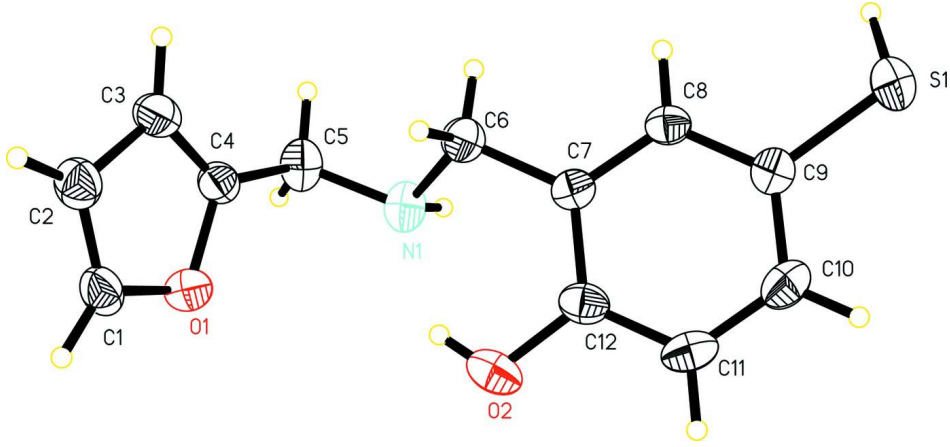

Figure 1

The molecular structure of (I) showing 30% probability displacement ellipsoids.

2-(2-Furylmethylaminomethyl)-4-sulfanylphenol

Crystal data

$C_{12}H_{13}NO_2S$
$M_r = 235.29$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.5778$ (12) Å
$b = 13.589$ (3) Å
$c = 14.943$ (3) Å
$V = 1132.6$ (4) Å^3
$Z = 4$
$F(000) = 496$
$D_x = 1.380$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9$–12°
$\mu = 0.27$ mm^{-1}
$T = 293$ K
Block, colorless
0.30 × 0.30 × 0.10 mm

Data collection

Enraf–Nonius CAD4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.924$, $T_{max} = 0.974$
2528 measured reflections
2216 independent reflections
1811 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.0°$
$h = -6\rightarrow0$
$k = -16\rightarrow16$
$l = -18\rightarrow0$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.166$
$S = 1.06$
2216 reflections
150 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1031P)^2 + 0.1612P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.058 (9)
Absolute structure: Flack (1983), 900 Friedel pairs
Absolute structure parameter: 0.00 (17)

Special details

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

	x	y	z	U_{iso}*/U_{eq}
C1	−0.2480 (7)	0.7259 (3)	0.4206 (3)	0.0591 (10)

H1	−0.3948	0.7288	0.4501	0.071*
C2	−0.1233 (8)	0.6441 (3)	0.4068 (3)	0.0581 (9)
H2	−0.1659	0.5807	0.4239	0.070*
C3	0.0881 (8)	0.6728 (3)	0.3607 (3)	0.0564 (10)
H3	0.2108	0.6312	0.3420	0.068*
C4	0.0791 (6)	0.7696 (3)	0.3490 (2)	0.0480 (8)
C5	0.2431 (8)	0.8424 (3)	0.3079 (3)	0.0600 (10)
H5A	0.2795	0.8933	0.3512	0.072*
H5B	0.3923	0.8100	0.2920	0.072*
C6	0.1385 (8)	0.8197 (2)	0.1507 (2)	0.0526 (9)
H6A	0.0551	0.7597	0.1671	0.063*
H6B	0.3023	0.8025	0.1354	0.063*
C7	0.0183 (6)	0.8652 (2)	0.0710 (2)	0.0422 (8)
C8	0.1130 (6)	0.8552 (2)	−0.0141 (2)	0.0449 (8)
H8	0.2558	0.8209	−0.0219	0.054*
C9	−0.0009 (7)	0.8953 (3)	−0.0874 (3)	0.0481 (8)
C10	−0.2099 (8)	0.9468 (3)	−0.0782 (3)	0.0591 (10)
H10	−0.2856	0.9737	−0.1280	0.071*
C11	−0.3069 (7)	0.9583 (3)	0.0062 (3)	0.0613 (11)
H11	−0.4480	0.9939	0.0134	0.074*
C12	−0.1958 (6)	0.9172 (3)	0.0804 (3)	0.0502 (9)
H1C	0.230 (9)	0.942 (3)	0.212 (3)	0.060*
N1	0.1391 (7)	0.8878 (2)	0.2275 (2)	0.0550 (8)
O1	−0.1310 (6)	0.8050 (2)	0.38570 (18)	0.0632 (8)
O2	−0.2984 (5)	0.9310 (2)	0.1623 (2)	0.0696 (8)
H2A	−0.2170	0.9038	0.2007	0.104*
S1	0.1282 (2)	0.88051 (8)	−0.19340 (6)	0.0635 (4)
H1A	0.3423	0.8770	−0.1863	0.095*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.041 (2)	0.091 (3)	0.0460 (19)	0.001 (2)	0.0025 (17)	0.011 (2)
C2	0.052 (2)	0.063 (2)	0.059 (2)	−0.006 (2)	0.005 (2)	0.0063 (17)
C3	0.053 (2)	0.058 (2)	0.057 (2)	0.0042 (18)	0.010 (2)	−0.0024 (18)
C4	0.0402 (19)	0.062 (2)	0.0419 (17)	0.0025 (16)	−0.0010 (15)	−0.0007 (16)
C5	0.058 (2)	0.068 (2)	0.054 (2)	−0.015 (2)	−0.007 (2)	0.0067 (19)
C6	0.055 (2)	0.0490 (18)	0.054 (2)	0.0003 (19)	0.002 (2)	0.0033 (16)
C7	0.0361 (17)	0.0396 (16)	0.0508 (19)	−0.0041 (15)	−0.0016 (15)	−0.0001 (14)
C8	0.0382 (17)	0.0426 (16)	0.0540 (19)	0.0009 (15)	0.0022 (17)	−0.0009 (14)
C9	0.047 (2)	0.0470 (18)	0.0501 (19)	−0.0058 (17)	−0.0034 (17)	0.0017 (15)
C10	0.054 (2)	0.057 (2)	0.066 (2)	0.0046 (19)	−0.017 (2)	0.0031 (19)
C11	0.041 (2)	0.060 (2)	0.083 (3)	0.0110 (17)	−0.007 (2)	−0.002 (2)
C12	0.0385 (19)	0.0486 (18)	0.064 (2)	−0.0037 (15)	0.0074 (17)	−0.0040 (17)
N1	0.064 (2)	0.0487 (16)	0.0518 (16)	−0.0126 (18)	−0.0062 (16)	0.0024 (14)
O1	0.0598 (17)	0.0678 (16)	0.0619 (16)	0.0180 (15)	0.0025 (15)	0.0038 (12)
O2	0.0543 (17)	0.0815 (18)	0.0731 (19)	0.0024 (15)	0.0224 (15)	−0.0063 (15)
S1	0.0710 (7)	0.0711 (7)	0.0486 (5)	−0.0030 (6)	0.0064 (5)	0.0029 (4)

Geometric parameters (Å, º)

C1—C2	1.328 (6)	C6—H6B	0.9700
C1—O1	1.361 (5)	C7—C8	1.383 (5)
C1—H1	0.9300	C7—C12	1.394 (5)
C2—C3	1.420 (6)	C8—C9	1.379 (5)
C2—H2	0.9300	C8—H8	0.9300
C3—C4	1.327 (5)	C9—C10	1.366 (6)
C3—H3	0.9300	C9—S1	1.752 (4)
C4—O1	1.381 (5)	C10—C11	1.382 (6)
C4—C5	1.481 (5)	C10—H10	0.9300
C5—N1	1.470 (5)	C11—C12	1.388 (6)
C5—H5A	0.9700	C11—H11	0.9300
C5—H5B	0.9700	C12—O2	1.365 (5)
C6—N1	1.473 (5)	N1—H1C	0.93 (5)
C6—C7	1.501 (5)	O2—H2A	0.8200
C6—H6A	0.9700	S1—H1A	1.2000
C2—C1—O1	110.5 (3)	C8—C7—C12	118.0 (3)
C2—C1—H1	124.8	C8—C7—C6	121.2 (3)
O1—C1—H1	124.8	C12—C7—C6	120.7 (3)
C1—C2—C3	106.3 (4)	C9—C8—C7	121.0 (3)
C1—C2—H2	126.8	C9—C8—H8	119.5
C3—C2—H2	126.8	C7—C8—H8	119.5
C4—C3—C2	107.7 (4)	C10—C9—C8	121.1 (4)
C4—C3—H3	126.1	C10—C9—S1	120.0 (3)
C2—C3—H3	126.1	C8—C9—S1	118.9 (3)
C3—C4—O1	108.9 (3)	C9—C10—C11	118.9 (4)
C3—C4—C5	133.9 (4)	C9—C10—H10	120.6
O1—C4—C5	117.2 (3)	C11—C10—H10	120.6
N1—C5—C4	112.1 (3)	C10—C11—C12	120.6 (4)
N1—C5—H5A	109.2	C10—C11—H11	119.7
C4—C5—H5A	109.2	C12—C11—H11	119.7
N1—C5—H5B	109.2	O2—C12—C11	118.3 (3)
C4—C5—H5B	109.2	O2—C12—C7	121.3 (4)
H5A—C5—H5B	107.9	C11—C12—C7	120.4 (4)
N1—C6—C7	111.1 (3)	C5—N1—C6	111.9 (3)
N1—C6—H6A	109.4	C5—N1—H1C	109 (3)
C7—C6—H6A	109.4	C6—N1—H1C	108 (2)
N1—C6—H6B	109.4	C1—O1—C4	106.5 (3)
C7—C6—H6B	109.4	C12—O2—H2A	109.5
H6A—C6—H6B	108.0	C9—S1—H1A	109.5
O1—C1—C2—C3	0.5 (5)	S1—C9—C10—C11	−179.4 (3)
C1—C2—C3—C4	−0.2 (5)	C9—C10—C11—C12	−0.8 (6)
C2—C3—C4—O1	−0.1 (4)	C10—C11—C12—O2	179.7 (4)
C2—C3—C4—C5	178.8 (4)	C10—C11—C12—C7	1.3 (6)
C3—C4—C5—N1	114.6 (5)	C8—C7—C12—O2	−179.2 (3)

O1—C4—C5—N1	−66.5 (4)	C6—C7—C12—O2	2.2 (5)
N1—C6—C7—C8	137.6 (3)	C8—C7—C12—C11	−0.8 (5)
N1—C6—C7—C12	−43.8 (5)	C6—C7—C12—C11	−179.4 (3)
C12—C7—C8—C9	−0.1 (5)	C4—C5—N1—C6	−73.9 (4)
C6—C7—C8—C9	178.6 (3)	C7—C6—N1—C5	176.6 (3)
C7—C8—C9—C10	0.5 (5)	C2—C1—O1—C4	−0.6 (4)
C7—C8—C9—S1	179.8 (3)	C3—C4—O1—C1	0.4 (4)
C8—C9—C10—C11	0.0 (6)	C5—C4—O1—C1	−178.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···N1	0.82	2.04	2.692 (5)	136
N1—H1*C*···S1^{i}	0.93 (5)	2.90 (4)	3.605 (3)	134 (3)

Symmetry code: (i) −*x*+1/2, −*y*+2, *z*+1/2.