Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 2-(2-Furylmethylaminomethyl)-4-sulfanylphenol

**Wu Chen, Lian Liu, Di Xu and Qing-Fu Zeng***

Engineering Research Center for Clean Production of Textile Dyeing and Printing, Ministry of Education, Wuhan 430073, People's Republic of China
Correspondence e-mail: qfzeng@wuse.edu.cn

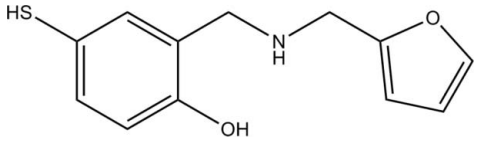
Received 14 August 2009; accepted 15 August 2009

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(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
$\mu$ = 0.27 mm$^{-1}$
$T$ = 293 K
0.30 × 0.30 × 0.10 mm

### *Data collection*

Enraf–Nonius CAD4 diffractometer
Absorption correction: $\psi$ 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—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) $-x+\frac{1}{2}, -y+2, z+\frac{1}{2}$.

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*.

The project was supported by the Scientific Research Foundation for Returned Overseas Chinese Scholars, State Education Ministry, Educational Commission of Hubei Province (D20091703) and the Natural Science Foundation of Hubei Province (2008CDB038).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5047).

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Enraf–Nonius (1989). *CAD-4 Software*. Enraf–Nonius, Delft, The Netherlands.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shi, L., Ge, H.-M., Tan, S.-H., Li, H.-Q., Song, Y.-C., Zhu, H.-L. & Tan, R.-X. (2007). *Eur. J. Med. Chem.* **42**, 558–564.

# supplementary materials

*Acta Cryst.* (2009). E**65**, o2204 [ **doi:10.1107/S1600536809032401** ]

# 2-(2-Furylmethylaminomethyl)-4-sulfanylphenol

**W. Chen, L. Liu, D. Xu and Q.-F. Zeng**

## 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).

## 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.

## 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) = 1.2$U_{eq}$(carrier) or 1.5$U_{eq}$(methyl C).

## Figures

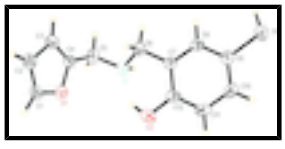


Fig. 1. The molecular structure of (I) showing 30% probability displacement ellipsoids.

## 2-(2-Furylmethylaminomethyl)-4-sulfanylphenol

*Crystal data*

| | |
|---|---|
| $C_{12}H_{13}NO_2S$ | $F_{000}$ = 496 |
| $M_r$ = 235.29 | $D_x$ = 1.380 Mg m$^{-3}$ |
| Orthorhombic, $P2_12_12_1$ | Mo $K\alpha$ radiation, λ = 0.71073 Å |
| Hall symbol: P 2ac 2ab | Cell parameters from 25 reflections |
| $a$ = 5.5778 (12) Å | θ = 9–12° |
| $b$ = 13.589 (3) Å | μ = 0.27 mm$^{-1}$ |

| | |
|---|---|
| $c$ = 14.943 (3) Å | $T$ = 293 K |
| $V$ = 1132.6 (4) Å$^3$ | Block, colorless |
| $Z$ = 4 | 0.30 × 0.30 × 0.10 mm |

*Data collection*

| | |
|---|---|
| Enraf–Nonius CAD4 diffractometer | $R_{int}$ = 0.034 |
| Radiation source: fine-focus sealed tube | $\theta_{max}$ = 26.0º |
| Monochromator: graphite | $\theta_{min}$ = 2.0º |
| $T$ = 293 K | $h$ = −6→0 |
| ω/2θ scans | $k$ = −16→16 |
| Absorption correction: ψ scan (North *et al.*, 1968) | $l$ = −18→0 |
| $T_{min}$ = 0.924, $T_{max}$ = 0.974 | 3 standard reflections |
| 2528 measured reflections | every 200 reflections |
| 2216 independent reflections | intensity decay: 1% |
| 1811 reflections with $I > 2\sigma(I)$ | |

*Refinement*

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

*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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, °)*

| | | | |
|---|---|---|---|
| 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, °)*

| *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 codes: (i) −*x*+1/2, −*y*+2, *z*+1/2.

**Fig. 1**