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# 3-(4-Fluorophenyl)-2-(4-methylphenoxy)-5,8,9-trimethylthieno[3′,2′:5,6]pyrido[4,3-*d*]pyrimidin-4(3*H*)-one

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**Key indicators**

Single-crystal X-ray study
*T* = 292 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.050
*wR* factor = 0.117
Data-to-parameter ratio = 16.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title molecule, $C_{25}H_{20}FN_3O_2S$, the central tricyclic system is essentially planar. All bond lengths and angles are within normal ranges. The crystal packing is stabilized by $\pi$–$\pi$ stacking interactions and van der Waals forces.

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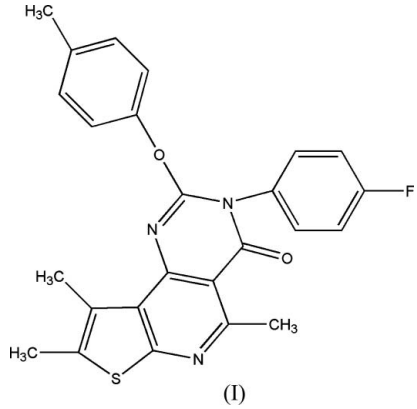
## Comment

Pyridine-containing heterocyclic compounds have been intensively studied due to the biological activity they often demonstrate (Augusto *et al.*, 1995). The title compound, (I), belongs to this family of heterocyclic compounds and we present its crystal structure here.




(I)

In (I) (Fig. 1), the C—S bond lengths [1.730 (2) and 1.744 (2) Å] are greater than those observed in free thiophene [**1.714 (s.u.) Å**; Bonham & Momany, 1963] and thieno[2,3-*c*]-pyridine [1.728 (1) and 1.731 (1) Å; Nerenz *et al.*, 1997]. The C5—S1—C6 angle of 91.29 (10)° in (I) is slightly less than that observed in free thiophene [92.2 (2)°]. As expected for a non-protonated ring system, the C1—N1—C9 angle of 117.17 (16)°

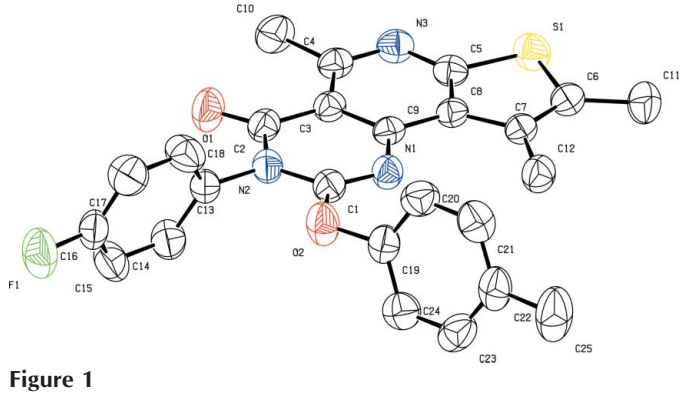



**Figure 1**
View of (I) showing the atom-labelling scheme and 50% probability displacement ellipsoids. H atoms have been omitted.

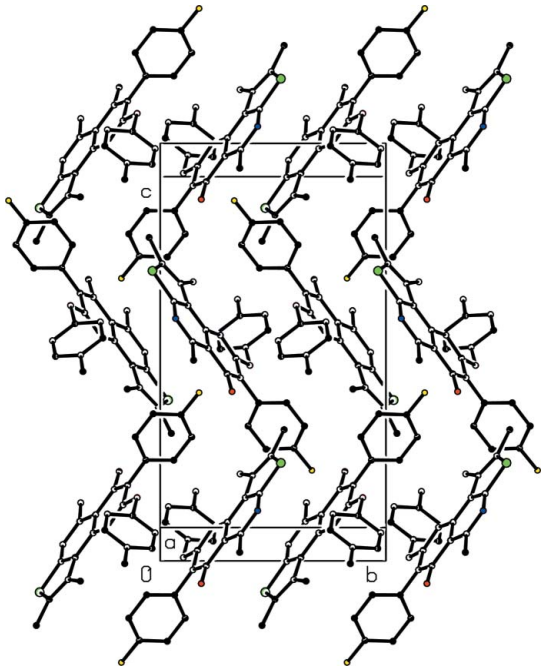



**Figure 2**
The crystal packing of (I), viewed approximately along the *a* axis. H atoms have been omitted.

is smaller than 120° (Ghosh & Simonsen, 1993). The torsion angles C4—C3—C9—N1 and C9—C8—C5—S1 are 179.41 (17) and 179.89 (13)°, respectively, showing the essential planarity of the tricyclic system. The short intermolecular distances between the centroids of the thiophene (*Cg*1), pyridine (*Cg*2) and pyrimidine (*Cg*3) rings [$Cg1\cdots Cg2^{i}$ = 3.525 (11) Å and $Cg1\cdots Cg3^{i}$ = 3.516 (12) Å; symmetry code: (i) $2-x, 1-y, -z$] indicate the existence of $\pi$–$\pi$ stacking interactions, which stabilize the crystal packing (Fig. 2) together with van der Waals forces.

## Experimental

To a solution of iminophosphorane (1 mmol) and 4-fluorophenyl isocyanate (1.1 mmol) in dry $CH_2Cl_2$ (20 ml) was added 4-methylphenol (1.1 mmol) and a catalytic amount of $K_2CO_3$ under $N_2$ at room temperature. After filtration, the solid was recrystallized from acetonitrile. Colourless block-shaped crystals of the title compound were obtained by evaporation of the solvent over a period of one week.

*Crystal data*

$C_{25}H_{20}FN_3O_2S$
$M_r$ = 445.50
Monoclinic, $P2_1/c$
$a$ = 11.0623 (10) Å
$b$ = 10.4086 (9) Å
$c$ = 20.2368 (15) Å
$\beta$ = 110.737 (4)°
$V$ = 2179.2 (3) Å$^3$
$Z$ = 4
$D_x$ = 1.358 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 2397 reflections
$\theta$ = 2.4–21.6°
$\mu$ = 0.19 mm$^{-1}$
$T$ = 292 (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.947, $T_{max}$ = 0.982
12598 measured reflections
4959 independent reflections
2909 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.054
$\theta_{max}$ = 27.5°
$h = -14 \rightarrow 9$
$k = -13 \rightarrow 13$
$l = -24 \rightarrow 26$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.117
$S$ = 0.89
4959 reflections
293 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0516P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

C-bound H atoms were introduced at calculated positions and refined using a riding model, with $U_{iso}$(H) = 1.2–1.5$U_{eq}$(C) and C—H = 0.93–0.96 Å.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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