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8-(4-Chlorophenoxy)-7-(4-chlorophenyl)-1,2,5-trimethylthieno[2′,3′;2,3]pyrido[4,5-*d*]pyrimidin-6(7*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 = 0.158
Data-to-parameter ratio = 16.4

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

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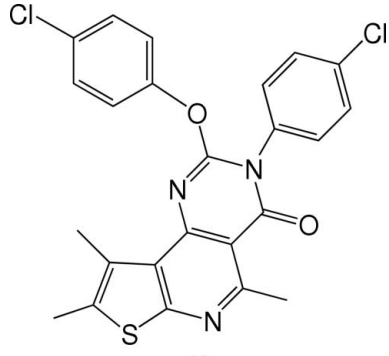
In the molecule of the title compound, $C_{24}H_{17}Cl_2N_3O_2S$, the mean plane of the tricyclic thienopyridopyrimidine system is roughly orthogonal to both benzene planes, the dihedral angles being 107.8 (1) and 99.6 (1)° for the benzene planes in the *p*-chlorophenoxy and *p*-chlorophenyl groups, respectively. The dihedral angle formed by the two benzene rings is 101.4 (1)°.

Comment

The derivatives of heterocyclic systems involving pyridine rings attract considerable interest because of their remarkable biological properties. Many pyridopyrimidines show biological activity and exhibit germicidal effects (Anderson & Broom, 1977). According to recent studies by Zheng *et al.* (2001), pyrimidine derivatives make up a novel class of adenosine kinase inhibitors. A large number of general methods for the preparation of pyridopyrimidine derivatives have been reported within the past few years (Rewcastle *et al.*, 1996; Maruoka *et al.*, 2004). Recently, we have developed a new and facile regioselective annulation process, which proceeds smoothly under mild conditions *via* a tandem aza–Wittig and cyclization reaction, and produces novel 8-substituted 1,2,5-trimethyl-7-phenylthieno[3′,2′;5,6]pyrido[4,3-*d*]pyrimidine-6(7*H*)-ones. In this paper, the crystal structure of the title compound, (I), is reported.



(I)

The molecular structure of (I) is shown in Fig. 1. Selected bond lengths and angles are listed in Table 1. In the molecule of the title compound, the mean plane of the tricyclic thienopyridopyrimidine 13-membered ring system S1/C2/C3/C5/C10/C9/C7/N1/C6/C12/N3/C11/N2 is roughly orthogonal to both benzene planes. The dihedral angles between the mean plane of the tricylic system and the benzene planes C13–C18 and C19–C24 are 99.6 (1)° and 107.8 (1)°, respectively; the benzene rings form a dihedral angle of 101.4 (1)°r.

Experimental

The title compound was prepared according to the literature procedure (Zhou *et al.*, 2005). Suitable crystals were obtained by evaporation of a methanol solution (m.p. > 573 K). Analysis calculated for $C_{24}H_{17}Cl_2N_3O_2S$: C 59.75, H 3.53, N 8.71%; found: C 60.11, H 3.66, N 8.52%.

Crystal data

$C_{24}H_{17}Cl_2N_3O_2S$	D_x = 1.448 Mg m^{-3}
M_r = 482.37	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3451 reflections
a = 11.1861 (17) Å	θ = 2.3–24.4°
b = 10.3346 (16) Å	μ = 0.42 mm^{-1}
c = 19.517 (3) Å	T = 292 (2) K
β = 101.377 (3)°	Block, colorless
V = 2212.0 (6) Å^3	0.35 × 0.30 × 0.30 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	4799 independent reflections
	3590 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.026
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)	θ_{max} = 27.0°
	$h = -14 \rightarrow 14$
T_{min} = 0.868, T_{max} = 0.885	$k = -13 \rightarrow 10$
12672 measured reflections	$l = -20 \rightarrow 24$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0852P)^2 + 0.2736P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.050	
$wR(F^2)$ = 0.158	
S = 1.10	$(\Delta/\sigma)_{max}$ = 0.001
4799 reflections	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
292 parameters	$\Delta\rho_{min}$ = −0.32 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C2—S1	1.733 (3)	C11—N2	1.277 (3)
C6—N1	1.327 (3)	C11—O2	1.343 (3)
C6—S1	1.736 (2)	C11—N3	1.366 (3)
C7—N1	1.333 (3)	C12—O1	1.199 (3)
C10—N2	1.379 (3)	C12—N3	1.421 (3)
C3—C2—C1	127.6 (2)	N1—C7—C8	115.5 (2)
C3—C2—S1	113.75 (18)	N2—C10—C5	117.6 (2)
C1—C2—S1	118.59 (19)	N2—C11—O2	121.4 (2)
N1—C6—C5	128.1 (2)	O2—C11—N3	112.24 (19)
N1—C6—S1	121.63 (17)	O1—C12—N3	118.7 (2)
C5—C6—S1	110.31 (18)	N3—C12—C9	113.70 (19)
N1—C7—C9	121.2 (2)		

The H atoms were constrained to ride on their parent atoms with C—H distances of 0.93–0.96 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ [$1.5U_{eq}(C)$ for methyl H atoms].

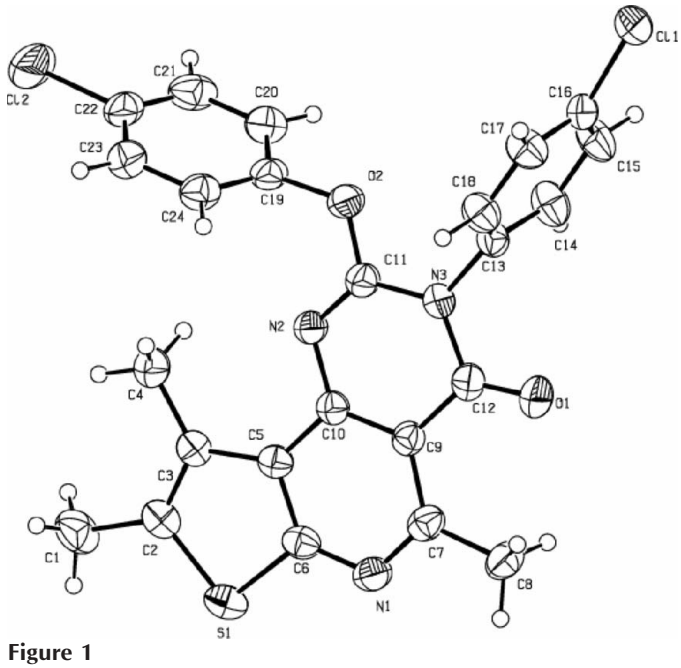


Figure 1
View of the molecule of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

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