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2-Ethoxy-3-phenyl-1-benzothieno[3,2-*d*]-pyrimidin-4(3*H*)-one

Sheng-Zhen Xu, Yang-Gen Hu, Xiang Wang and Ming-Wu Ding*

Key Laboratory of Pesticides and Chemical Biology of the Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China

Correspondence e-mail:
ding2005711@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.120
Data-to-parameter ratio = 17.3

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

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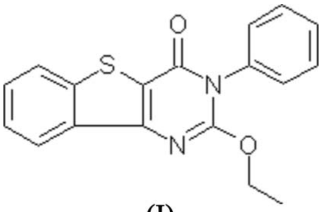
In the crystal structure of the title compound, $C_{18}H_{14}N_2O_2S$, the packing of the molecules is mainly governed by intermolecular π–π interactions.

Comment

Derivatives of thienopyrimidines are of great importance because of their remarkable biological properties (Walter, 1999*a*,*b*). In recent years, we have been engaged in the preparation of heterocyclic derivatives containing a fused pyrimidinone system using the aza-Wittig reaction (Ding *et al.*, 2004). Some X-ray crystal structure reports for thienopyrimidine derivatives have been published (Xu *et al.*, 2005; Cao *et al.*, 2006). Here, the structure of the title compound, (I), which may be used as a new precursor for obtaining bioactive molecules, is reported (Fig. 1).



(I)

The benzothienopyrimidine ring system is almost planar, with a maximum deviation of 0.042 (2) Å for atom C3; the C11–C16 phenyl ring is twisted with respect to it, with a dihedral angle of 58.38 (6)°. Intermolecular π–π interactions seem to be effective in stabilizing the crystal structure (Fig. 2). The centroid–centroid distances between the S1/C6/C1/C7/C8 and C1–C6 rings, and between the N1/C7–C9/N2/C10 and C1–C6 rings are 3.777 (1) and 3.644 (1) Å, respectively [interplanar distances 3.540 (1) and 3.518 (1) Å, respectively]. There are no inter- or intramolecular hydrogen-bonding interactions.

Experimental

To a solution of ethyl 3-(triphenylphosphoranylideneamino)benzo-[*b*]thiophene-2-carboxylate (3 mmol) in dry dichloromethane (5 ml) was added phenyl isocyanate (3 mmol) under nitrogen at room temperature. After the reaction mixture was left to stand for 10 h at 273–278 K, the solvent was removed under reduced pressure and diethyl ether/petroleum ether (1:2, 12 ml) was added to precipitate triphenylphosphine oxide. After filtration, anhydrous ethanol (10 ml) was added with several drops of EtONa in EtOH. The mixture was stirred for 6 h at room temperature. The solution was then concentrated under reduced pressure and the residue was recrystallized from ethanol to afford compound (I) (yield 58%, m.p. 463 K).

Suitable crystals were obtained by vapour diffusion of ethanol into dichloromethane at room temperature.

Crystal data

$C_{18}H_{14}N_2O_2S$
$M_r = 322.37$
Monoclinic, $C2/c$
$a = 22.4877$ (18) Å
$b = 11.2298$ (9) Å
$c = 14.8969$ (12) Å
$\beta = 126.298$ (1)°
$V = 3031.9$ (4) Å^3
$Z = 8$
$D_x = 1.412$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.23$ mm^{-1}
$T = 292$ (2) K
Block, colorless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{\min} = 0.936$, $T_{\max} = 0.956$
16980 measured reflections
3620 independent reflections
3090 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.057$
$\theta_{\max} = 28.0$°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.120$
$S = 1.05$
3620 reflections
209 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0671P)^2 + 0.7743P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.21$ e Å^{-3}
$\Delta\rho_{\min} = -0.35$ e Å^{-3}

H atoms were located in a difference map and treated as riding, with C—H = 0.93–0.98 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or $1.5U_{\rm eq}$(methyl C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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: *SHELXTL* (Sheldrick, 2001).

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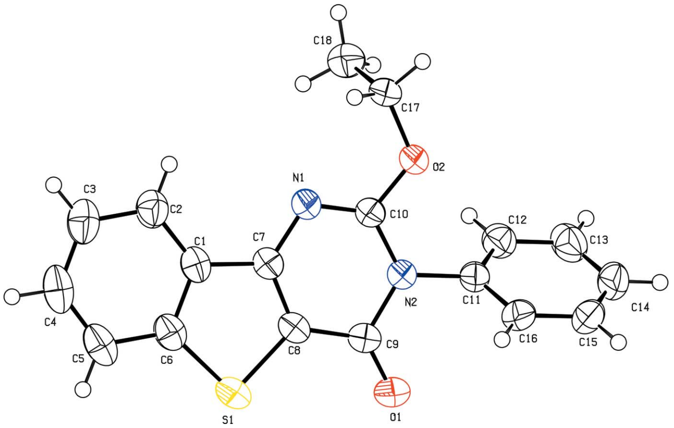

Figure 1
View of the molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

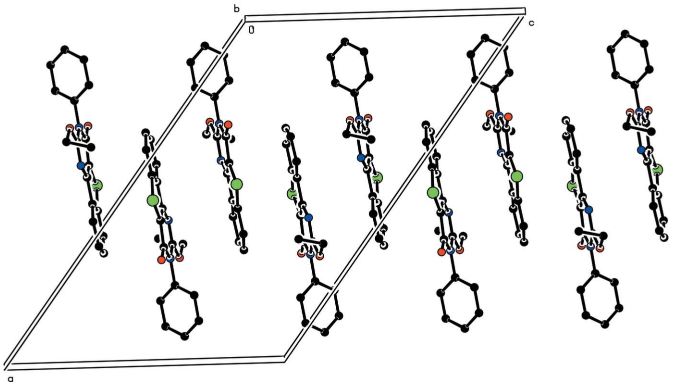

Figure 2
The crystal structure of (I), viewed along the *b* axis. H atoms bonded to C atoms have been omitted for clarity.

References

Bruker (2001). *SMART* (Version 5.628) and *SAINT* (Version 6.45). Bruker AXS Inc., Madison, Wisconsin, USA.

Cao, M.-H., Xu, S.-Z. & Hu, Y.-G. (2006). *Acta Cryst.* E**62**, o1319–o1320.

Ding, M.-W., Xu, S.-Z. & Zhao, J.-F. (2004). *J. Org. Chem.* **69**, 8366–8371.

Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.

Sheldrick, G. M. (2001). *SHELXTL*. Version 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (2003). *SADABS*. Version 2.10. Bruker AXS inc., Madison, Wisconsin, USA.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Walter, H. (1999*a*). PCT Int. Appl. No. 44.

Walter, H. (1999*b*). PCT Int. Appl. No. 89.

Xu, S.-Z., Cao, M.-H., Hu, Y.-G., Ding, M.-W. & Xiao, W.-J. (2005). *Acta Cryst.* E**61**, o2789–o2790.

o2230 Xu *et al.* • $C_{18}H_{14}N_2O_2S$ *Acta Cryst.* (2006). E**62**, o2229–o2230