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2-(4,6-Dimethoxypyrimidin-2-ylsulfanyl)-*N*-phenylbenzamide

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Key indicators

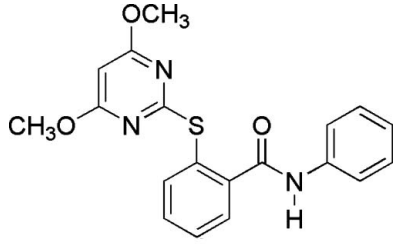
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.033
wR factor = 0.072
Data-to-parameter ratio = 17.4

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

The title compound, $C_{19}H_{17}N_3O_3S$, was synthesized *via* the reaction of 2-(4,6-dimethoxypyrimidin-2-ylsulfanyl)benzoic acid and aniline in dichloromethane using dicyclohexylcarbodiimide as catalyst. The dihedral angles between the pyrimidine plane and the planes of the two benzene rings are 71.2 (2) and 62.7 (2)°; the dihedral angle between the planes of the two benzene rings is 68.4 (4)°. The conformation of the compound is U-shaped.

Comment

2-(4,6-Dimethoxypyrimidin-2-ylthio)benzoic acid derivatives have been found to exhibit herbicidal activity against grasses and broadleaf weeds over a wide range of growth stages (Nezu *et al.*, 1996; Luthy *et al.*, 2001).



(I)

The molecular structure of the title compound, (I), is shown in Fig. 1. The bond lengths and angles are unexceptional. Those in the pyrimidine ring are similar to the values found in a related compound (Wu *et al.*, 2003). The pyrimidine ring makes dihedral angles of 62.7 (2) and 71.2 (2)° with the C7–C12 and C14–C19 benzene rings, respectively. The dihedral angle between the planes of the two benzene rings is 68.4 (4)°.

Hydrogen-bonding interactions plays an important role in the solid-state structure of (I) (Table 1). These lead to the formation of chains parallel to the *a* axis.

Experimental

To a mixture of 2-(4,6-dimethoxypyrimidin-2-ylsulfanyl)benzoic acid (13.0 g, 44.0 mmol) and aniline (13.8 g, 39mmol) in dichloromethane (30 ml), a solution of dicyclohexylcarbodiimide (8.8 g, 44 mmol) in dichloromethane (80 ml) was added dropwise over a period of 20 min. The mixture was stirred for 6 h at room temperature. The solid was filtered off and washed with dichloromethane (20 ml). The filtrate was treated with 10% sodium hydroxide (50 ml), stirred for 1 h and extracted with dichloromethane (2 × 30 ml). The organic layer was separated, dried with magnesium sulfate and evaporated in vacuo to give a crude product as white powder. After 5 d, single crystals suitable for X-ray analysis were obtained by recrystallization from ethanol.

Crystal data

$C_{19}H_{17}N_3O_3S$
M_r = 367.42
Orthorhombic, *Pbca*
a = 9.3750 (1) Å
b = 14.4845 (2) Å
c = 26.4390 (3) Å
V = 3590.21 (7) Å^3
Z = 8
D_x = 1.359 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 30626 reflections
θ = 2.2–27.5°
μ = 0.20 mm^{-1}
T = 295 (1) K
Block, colourless
0.31 × 0.20 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.868, T_{max} = 0.972
31250 measured reflections
4111 independent reflections
2299 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.041
θ_{max} = 27.5°
$h = -11 \rightarrow 12$
$k = -18 \rightarrow 18$
$l = -34 \rightarrow 34$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.072
S = 1.00
4111 reflections
236 parameters
H-atom parameters constrained
$w = 1/[0.0002F_o^2 + 0.9\sigma(F_o^2)]/(4F_o^2)$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Extinction correction: Larson (1970), equation 22
Extinction coefficient: 131 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H301···O3^{i}	0.86	2.11	2.916 (1)	156

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

H atoms were placed in calculated positions, with C—H = 1.00 Å (CH) or 0.96 Å (methyl) and N—H = 0.86 Å, and included in the final cycles of refinement in the riding model, with U_{iso}(H) = 1.2U_{eq}(carrier atom).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

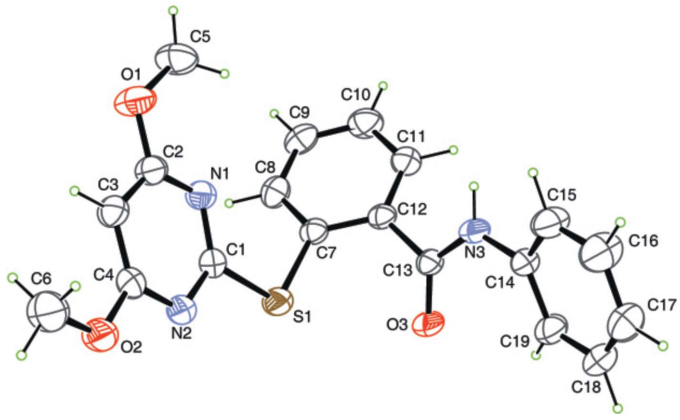


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 40% probability level.

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References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, C. K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Larson, A. C. (1970). *Crystallographic Computing*, edited by F. R. Ahmed, S. R. Hall & C. P. Huber, pp. 291–294. Copenhagen: Munksgaard.
Luthy, C., Zondler, H., Rapold, T., Seifert, G., Urwyler, B., Heinis, T., Steinrucken, H. C. & Allen, J. (2001). *Pest Manag. Sci.* **57**, 205–224.
Nezu, Y., Wada, N., Saitoh, Y., Takahashi, S. & Miyazawa, T. (1996). *J. Pestic. Sci.* **21**, 293–303.
Rigaku (1998). *PROCESS-AUTO*. Version 1.06. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2004). *CrystalStructure*. Version 3.6.0. Rigaku/MSC, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
Wu, J., Zhang, P. Z., Yu, Q. S., Hu, X. R. & Gu, J. M. (2003). *Acta Cryst.* E**59**, o1393–o1394.