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2-Amino-4,6-bis(phenylthio)pyrimidine

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Key indicators

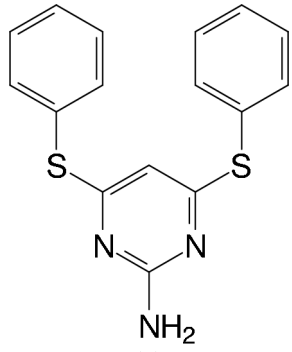
Single-crystal X-ray study
T = 151 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.117
Data-to-parameter ratio = 17.6

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

The structure of the title compound, $C_{16}H_{13}N_3S_2$, (I), consists of molecules that associate *via* N—H···N and N—H···S interactions to form a linear one-dimensional hydrogen-bonded chain. The dihedral angles between the two phenyl rings and the pyrimidine ring are 74.94 (7) and 75.47 (7)°.

Experimental

The title compound, (I), was prepared by Spa Contract Synthesis. Crystals of (I) were grown from DMF/methanol (1/10) solution.



(I)

Crystal data

$C_{16}H_{13}N_3S_2$
M_r = 311.41
Monoclinic, $P2_1/n$
a = 8.7937 (18) Å
b = 8.3091 (17) Å
c = 21.148 (4) Å
β = 95.73 (3)°
V = 1537.5 (5) Å^3
Z = 4
D_x = 1.345 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6016 reflections
θ = 1.0–27.5°
μ = 0.34 mm^{-1}
T = 150 (2) K
Block, colourless
0.34 × 0.18 × 0.16 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.893, T_{max} = 0.947
12 370 measured reflections
3476 independent reflections
2440 reflections with $I > 2\sigma(I)$
R_{int} = 0.088
θ_{max} = 27.5°
$h = -11 \rightarrow 10$
$k = -9 \rightarrow 10$
$l = -27 \rightarrow 27$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.117
S = 1.00
3476 reflections
198 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0595P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.009
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N21—H21···N3^{i}	0.78 (2)	2.32 (2)	3.102 (2)	177 (2)
N21—H22···S2^{ii}	0.90 (2)	2.88 (2)	3.586 (2)	136.2 (17)

Symmetry codes: (i) $-1-x, 2-y, -z$; (ii) $-x, 2-y, -z$.

All H atoms were included in the refinement, at calculated positions, as riding models with C—H set to 0.95 Å (Ar-H), except for the amine H atoms, which were located on difference syntheses and both positional and thermal parameters refined.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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