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1,3-Bis(pyrimidin-2-ylsulfanyl)propan-2-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.062
wR factor = 0.106
Data-to-parameter ratio = 10.7

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

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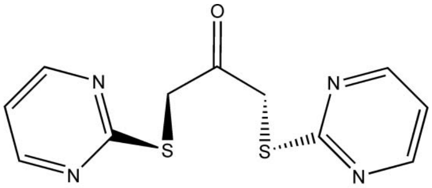
The title compound, $C_{11}H_{10}N_4OS_2$, has a twofold axis passing through the carbonyl group. The molecules stack along the *b* axis *via* π–π interactions.

Comment

In recent years, N-containing heterocyclic thioethers linked by various aryl or alkyl groups have been widely exploited in metal-organic self-assembly as multitopic bridging ligands, and several unique structural motifs with this type of ligand have been obtained (Hong *et al.*, 2000; Zheng *et al.*, 2003). Thus, we designed and synthesized the title compound, (I), which is a new nitrogen-containing heterocyclic thioether ligand with a propan-2-one moiety as the linkage.



(I)

In (I), there is a twofold rotation axis passing through the C6═O1 carbonyl group of the propanone moiety (Fig. 1). Two pyrimidin-2-ylsulfanyl groups are oriented *anti* with respect to the propanone moiety. Atom S1 deviates from the least-squares plane of atoms C5/C5^i/C6/O1 by 0.806 (1) Å [symmetry code: (i) $1 - x, y, \frac{3}{2} - z$]. The dihedral angle between the two pyrimidine rings is 48.1 (1)°, while that between the propanone moiety and the pyrimidine ring is 78.3 (1)°. Notably, the molecules stack along the *b* axis through π–π interactions, with center-to-center distances of 3.662 Å (Fig. 2).

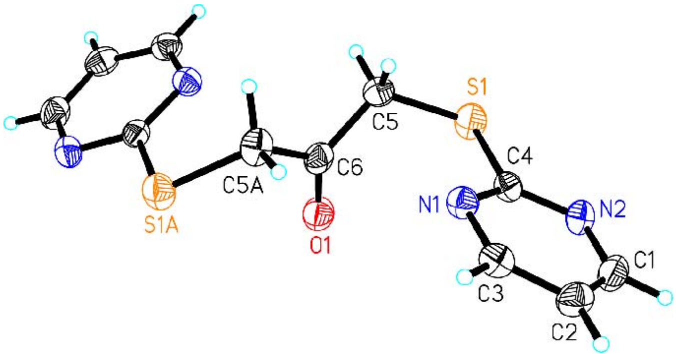


Figure 1
Perspective view of (I), showing the atom-numbering scheme. Displacement ellipsoids are shown at the 30% probability level. [Symmetry code: (A) $1 - x, y, \frac{3}{2} - z$.]

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Experimental

Sodium methoxide (0.540 g, 10 mmol) and 2-mercaptopyrimidine (1.12 g, 10 mmol) were stirred vigorously in MeOH (50 ml) for 1 h; a quantitative amount of 1,3-dichloro-2-propanone (0.635 g, 5 mmol) was then added. The resulting solution was heated at 373 K for 12 h and filtered after cooling to room temperature. Removal of the solvent from the yellow filtrate yielded a yellow powder which was washed with water and recrystallized from methanol to produce yellow crystals of (I) (yield 1.01 g, 72%). Slow evaporation of a methanol solution of (I) over a period of two weeks yielded yellow prism-shaped crystals suitable for X-ray diffraction.

Crystal data

$C_{11}H_{10}N_4OS_2$
$M_r = 278.35$
Orthorhombic, *Pbcn*
$a = 7.8042\ (11)$ Å
$b = 7.3159\ (11)$ Å
$c = 21.753\ (3)$ Å
$V = 1242.0\ (3)$ Å^3
$Z = 4$
$D_x = 1.489$ Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 6883 reflections
$\theta = 1.9$–25.0°
$\mu = 0.42$ mm^{-1}
$T = 293\ (2)$ K
Prism, yellow
0.12 × 0.10 × 0.06 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.775$, $T_{\max} = 0.975$
6883 measured reflections

1101 independent reflections
813 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.075$
$\theta_{\max} = 25.0^\circ$
$h = -9 \rightarrow 9$
$k = -8 \rightarrow 8$
$l = -25 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.106$
$S = 1.15$
1101 reflections
103 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0245P)^2 + 1.036P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C4	1.759 (3)	O1—C6	1.212 (6)
S1—C5	1.793 (4)		
C4—S1—C5	99.86 (18)	O1—C6—C5	123.3 (3)
C6—C5—S1	114.8 (3)	C5—C6—C5$^{\rm i}$	113.4 (5)
C5—S1—C4—N1	2.1 (3)	S1—C5—C6—O1	−29.7 (3)
C4—S1—C5—C6	−64.2 (3)	S1—C5—C6—C5$^{\rm i}$	150.3 (3)

Symmetry code: (i) $1 - x, y, \frac{3}{2} - z$.

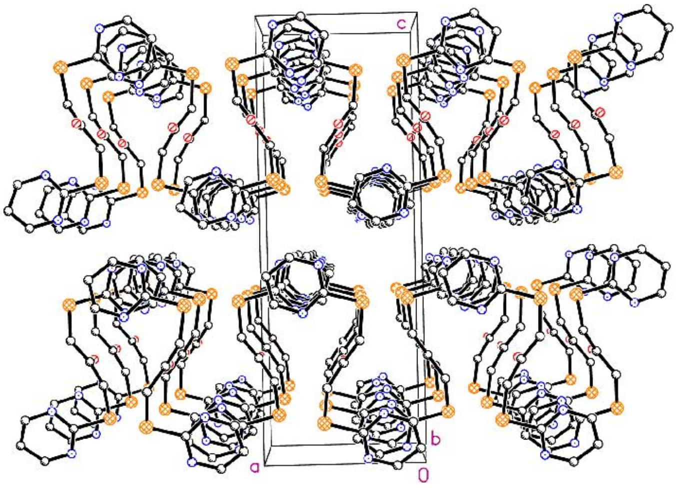

Figure 2
Packing diagram of (I), projected along the *b* axis, showing the stacked arrangement of molecules. H atoms have been omitted.

All H atoms were located in difference Fourier maps and their positional and isotropic displacement parameters were refined. The C—H bond lengths are 0.91 (3)–1.00 (4) Å.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *SAINT* and *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXL97*.

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