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Key indicators

Single-crystal X-ray study

T = 293 K

Mean $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$

R factor = 0.088

wR factor = 0.307

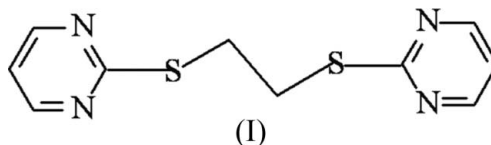
Data-to-parameter ratio = 18.4

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

1,2-Bis(pyrimidin-2-ylsulfanyl)ethane

The title dithioether compound, $\text{C}_{10}\text{H}_{10}\text{N}_4\text{S}_2$, adopts an *anti* conformation with an intramolecular $\text{S}\cdots\text{S}$ non-bonding distance of 4.419 (2) Å. The dihedral angle between the two pyrimidine rings is 6.8 (2)°.

Comment

A large number of complexes of dithioether ligands containing *N*-heterocyclic groups have been synthesized and investigated, because of their diverse coordination capabilities and the important properties of their metal complexes (Zheng *et al.*, 2003; Hong *et al.*, 2000). However, crystallographic studies of only a few ligands have been reported. In the present paper, we report the crystal structure of the title compound, (I).

As shown in Fig. 1, the molecule adopts an *anti* conformation (Goodgame *et al.*, 1999) with a pseudo-torsion angle $\text{C4}-\text{S1}\cdots\text{S2}-\text{C7}$ of $-174.9 (2)^\circ$. The pyrimidine rings ($\text{N1}/\text{C1}-\text{C3}/\text{N2}/\text{C4}$ and $\text{N3}/\text{C7}/\text{N4}/\text{C8}-\text{C10}$), with a dihedral angle of $6.8 (2)^\circ$ to each other, incline to the spacer unit plane ($\text{S1}-\text{C5}-\text{C6}-\text{S2}$) at angles of $81.8 (4)$ and $86.9 (4)^\circ$, respectively. The $\text{S1}\cdots\text{S2}$ non-bonding distance is 4.419 (2) Å. The bond dimensions are within the range reported in a similar compound, 2,4,6-trimethyl-1,3,5-tris(2-pyrimidinylthiomethyl)benzene (Zheng *et al.*, 2002). Both the $\text{S}-\text{Csp}^2$ and the $\text{S}-\text{Csp}^3$ bond distances of (I) show little deviation in comparison with those of the analogous compound 1,2-bis(phenylthio)ethane (Hou *et al.*, 2005), despite different substituents. The molecule of (I) does not possess any crystallographic symmetry, in contrast with the inversion symmetry of several reported alkyl dithioether compounds (Chen *et al.*, 2005; Hou *et al.*, 2005).

In the crystal structure of the binuclear silver(I) nitrate complex with (I) as a chelating and bridging ligand (Zheng *et al.*, 2003), the thioether adopts a *gauche* conformation with an $\text{S}\cdots\text{S}$ non-bonding distance of 3.44 (3) Å.

Experimental

Compound (I) was prepared according to the reported procedure (Zheng *et al.*, 2003). Colourless single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a chloroform solution at room temperature.

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Crystal data

$C_{10}H_{10}N_4S_2$
 $M_r = 250.34$
 Monoclinic, $P2_1/c$
 $a = 8.0524$ (16) Å
 $b = 19.884$ (4) Å
 $c = 8.1541$ (16) Å
 $\beta = 116.57$ (3)°
 $V = 1167.7$ (4) Å³
 $Z = 4$

$D_x = 1.424$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 11145 reflections
 $\theta = 3.0$ – 27.5 °
 $\mu = 0.43$ mm⁻¹
 $T = 293$ (2) K
 Needle, colourless
 $0.79 \times 0.24 \times 0.16$ mm

Data collection

Rigaku X-Axis RAPID IP area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.725$, $T_{\max} = 0.936$
 11145 measured reflections

2663 independent reflections
 1706 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.080$
 $\theta_{\text{max}} = 27.5$ °
 $h = -10 \rightarrow 10$
 $k = -25 \rightarrow 25$
 $l = -9 \rightarrow 10$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.088$
 $wR(F^2) = 0.307$
 $S = 1.02$
 2663 reflections
 145 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.2005P)^2 + 0.4011P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.046$
 $\Delta\rho_{\text{max}} = 1.17$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.94$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

S1–C4	1.759 (4)	S2–C7	1.757 (4)
S1–C5	1.866 (7)	S2–C6	1.939 (6)
C4–S1–C5	102.6 (2)	C7–S2–C6	102.24 (19)
C5–S1–C4–N2	7.7 (4)	C7–S2–C6–C5	88.1 (4)
C4–S1–C5–C6	–83.4 (4)	C6–S2–C7–N4	–12.1 (4)
S1–C5–C6–S2	–179.0 (2)		

All H atoms were positioned geometrically with $Csp^2-H = 0.93$ Å and $Csp^3-H = 0.97$ Å; they were constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The short C5–C6 distance of 1.425 (7) Å may be an artifact of unresolved disorder, in view of the large atomic displacements. The highest residual electron-density peak is 0.96 Å from atom C5.

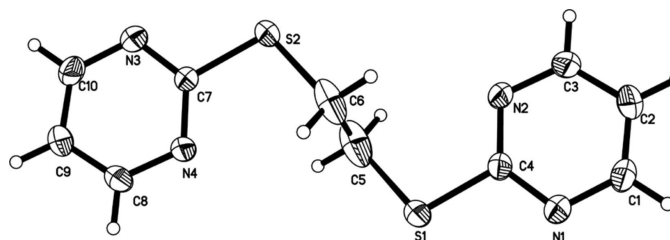


Figure 1

ORTEP (Johnson, 1976) view of (I), showing atomic displacement ellipsoids at the 30% probability level.

Data collection: RAPID-AUTO (Rigaku, 2004); cell refinement: RAPID-AUTO; data reduction: RAPID-AUTO; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP (Johnson, 1976); software used to prepare material for publication: CrystalStructure (Rigaku, 2004).

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