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4-Chloro-2-methylthio-6-(1-piperidyl)pyrimidine

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Key indicators

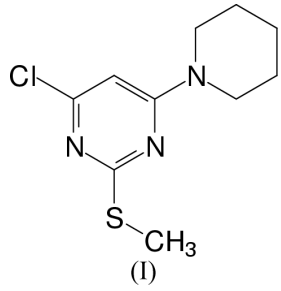
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.116
Data-to-parameter ratio = 18.8

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, $C_{10}H_{14}ClN_3S$, comprises a non-planar molecule with only one intramolecular close-contact association between a piperidinyl C—H group and a pyrimidine N atom. The pyrimidine–methylthio torsion angle is 5.7 (2)°.

Comment

The title compound, (I), was prepared from 4,6-dichloro-2-methylthiopyrimidine. Both Cl atoms can be displaced by nucleophiles before the methylthio group but the reactivity of the second Cl atom is much less than the first. This difference in reaction rate can be used to prepare unsymmetrical 4,6-substituted 2-methylthiopyrimidines because the product of the loss of the first Cl atom can be separated in large yield, *e.g.* compound (I). An interesting feature of the structure of 4,6-dichloro-2-methylthiopyrimidine is that there are six unique molecules in the asymmetric unit (Lynch & McClenaghan, 2000), differences arising due to the out-of-plane twist the methylthio bond makes with respect to the pyrimidine ring. The structure determination of the title compound was undertaken within a study of the effects that different substituents of 2-methylthiopyrimidines have on the pyrimidine–methylthio torsion angle.



(I)

Experimental

The title compound, (I), was prepared by Spa Contract Synthesis. Crystals of (I) were grown from an ethanol solution.

Crystal data

$C_{10}H_{14}ClN_3S$
M_r = 243.75
Orthorhombic, *Pbca*
a = 13.189 (3) Å
b = 8.577 (2) Å
c = 20.195 (4) Å
V = 2284.4 (8) Å^3
Z = 8
D_x = 1.417 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 15 006 reflections
θ = 2.9–30.5°
μ = 0.49 mm^{-1}
T = 150 (2) K
Block, colourless
0.40 × 0.40 × 0.36 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.829, T_{max} = 0.844
11 709 measured reflections
2580 independent reflections
2124 reflections with $I > 2\sigma(I)$
R_{int} = 0.070
θ_{max} = 27.5°
$h = -17 \rightarrow 17$
$k = -11 \rightarrow 10$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.117
S = 1.06
2580 reflections
137 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2 + 0.3268P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected geometric parameters (°).

N1—C2—S2—C21	5.7 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C66—H661···N1	0.99	2.30	2.744 (2)	106

All H atoms were included in the refinement at calculated positions as riding models with C—H set to 0.95 (Ar-H), 0.98 (CH_3) and 0.99 Å (CH_2). The methyl group was allowed to rotate about its local threefold axis.

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.

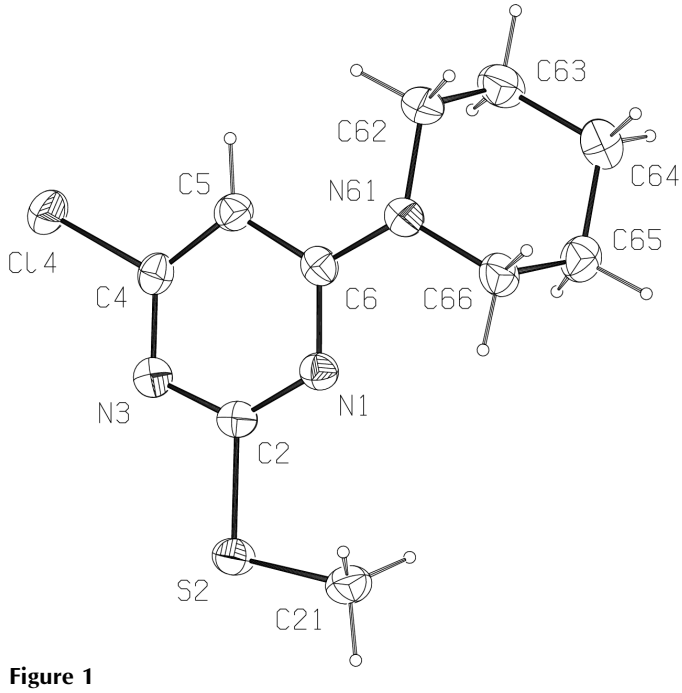


Figure 1
The molecular configuration and atom-numbering scheme for (I) showing 50% probability ellipsoids.

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