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4,6-Dichloro-2-(methylthio)-pyrimidine

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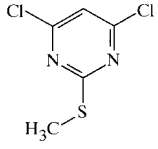
The structure of the title compound, $C_{30}H_{24}Cl_{12}N_{12}S_6$, (I), comprises six symmetry unique molecules that vary only slightly in their N—C—S—C torsion angle. All the molecules are planar to within less than 3.1°.



(I)

Experimental

Crystals of (I) were obtained from Spa Contract Synthesis.

Crystal data

$C_5H_4Cl_2N_2S$
M_r = 195.07
Triclinic, $P\overline{1}$
a = 13.6482 (2) Å
b = 14.1294 (2) Å
c = 14.1343 (2) Å
α = 119.9578 (7)°
β = 95.9391 (6)°
γ = 92.8349 (7)°
V = 2332.60 (6) Å^3
Z = 12
D_x = 1.666 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 15842 reflections
θ = 2.91–27.48°
μ = 1.022 mm^{-1}
T = 150 (2) K
Block, yellow
0.30 × 0.13 × 0.13 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.749, T_{max} = 0.883
34 427 measured reflections
10 671 independent reflections
8028 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.48°
$h = -17 \rightarrow 17$
$k = -18 \rightarrow 18$
$l = -18 \rightarrow 18$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.099
S = 1.042
10 671 reflections
547 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 0.2046P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.029
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Table 1
Selected geometric parameters (°).

N1*A*—C2*A*—S21*A*—C22*A*	−2.21 (16)
N1*B*—C2*B*—S21*B*—C22*B*	0.11 (16)
N1*C*—C2*C*—S21*C*—C22*C*	3.07 (16)
N1*D*—C2*D*—S21*D*—C22*D*	−1.92 (16)
N1*E*—C2*E*—S21*E*—C22*E*	2.69 (16)
N1*F*—C2*F*—S21*F*—C22*F*	−0.30 (17)

All H atoms were included in the refinement at calculated positions as riding, with th C—H distance set to either 0.98 (for methyl H atoms) or 0.95 Å (for aryl H atoms).

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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