Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2*E*)-2-(2,4-Dichlorobenzylidene)-6,7-dihydro-2*H*-thiazolo[3,2-*a*]pyrimidin-3(5*H*)-one

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Received 28 June 2004
Accepted 7 July 2004
Online 17 July 2004

Key indicators

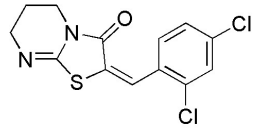
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.094
Data-to-parameter ratio = 16.5

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

The title compound, $C_{13}H_{10}Cl_2N_2OS$, was synthesized by mixing 2,4-dichlorobenzaldehyde, ethyl chloroacetate and tetrahydropyrimidine-2-thione in ethanol. The nearly planar thiazoline ring is fused to a dihydropyrimidine ring, which has a sofa conformation. The molecules are connected through weak C—H···N, C—H···O and C—H···Cl interactions.

Comment

The title molecule, (I) (Fig. 1), except for atom C2 and the H atoms, is planar to within 0.015 (3) Å, with C2 lying 0.601 (2) Å out of the plane, such that the dihydropyrimidine ring has a sofa conformation. Molecules are connected by weak C—H···N, C—H···O and C—H···Cl interactions (Fig. 2), with C···O = 3.349 (2) Å and C—H···O = 154°, C···N = 3.291 (2) Å and C—H···N = 174°, and C···Cl = 3.711 (2) Å and C—H···Cl = 163°.



(I)

Experimental

A mixture of tetrahydropyrimidine-2-thione (0.02 mol), ethyl chloroacetate (0.02 mol) and pyridine (0.02 mol) was stirred under reflux in ethanol (40 ml) for 4 h. 2,4-Dichlorobenzaldehyde (0.02 mol) and piperidine (0.02 mol) were then added and the mixture was refluxed for 4 h. After cooling and filtration, the title compound was recrystallized from acetic acid (m.p. 437–439 K). ^{1}H NMR (p.p.m.): 1.18 (*m*, 1H, $-CH_2$), 1.66 (*m*, 1H, $-CH_2$), 3.31 (*m*, 2H, $-CH_2$), 6.11 (*s*, 1H, —CH), 7.24–7.51 (*m*, 3H, ArH), 7.76 (*s*, 1H, —CH). 15 mg of (I) was dissolved in 15 ml trichloromethane and the solution was kept at room temperature for 7 d. Natural evaporation gave yellow needles of (I), suitable for X-ray analysis.

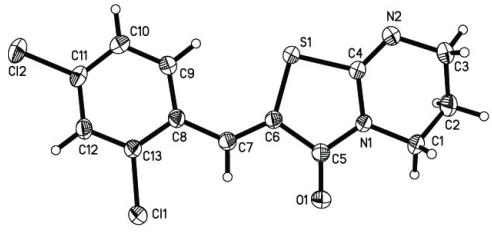


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

Crystal data

$C_{13}H_{10}Cl_2N_2OS$	D_x = 1.555 Mg m^{-3}
M_r = 313.19	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 791 reflections
a = 6.155 (2) Å	θ = 3.6–26.5°
b = 9.676 (4) Å	μ = 0.63 mm^{-1}
c = 22.507 (8) Å	T = 293 (2) K
β = 93.543 (6)°	Block cut from needle, yellow
V = 1337.8 (8) Å^3	0.28 × 0.26 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	2841 independent reflections
φ and ω scans	2191 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	R_{int} = 0.025
T_{min} = 0.820, T_{max} = 0.881	θ_{max} = 26.8°
7749 measured reflections	$h = -7 \rightarrow 7$
	$k = -12 \rightarrow 12$
	$l = -19 \rightarrow 28$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0406P)^2 + 0.4345P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.038	
$wR(F^2)$ = 0.094	
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.001
2841 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
172 parameters	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
H-atom parameters constrained	

The H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and refined in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

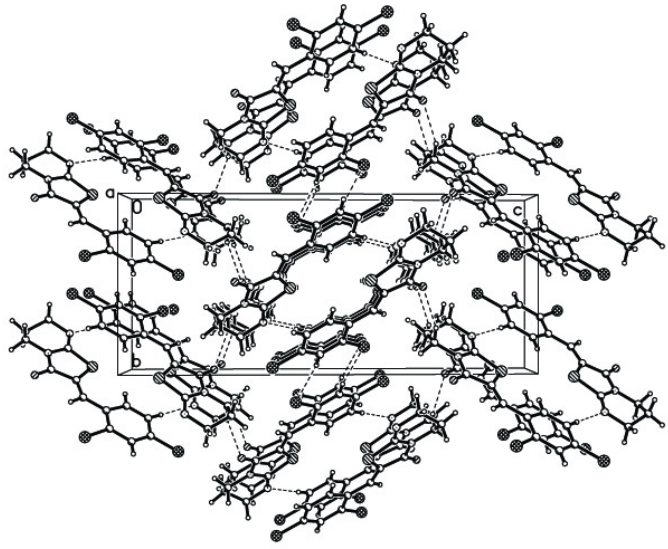


Figure 2
The crystal structure of (I), viewed along the *a* axis. Weak intermolecular interactions are shown as dashed lines.

References

Bruker (1997). *SADABS, SMART, SAINT* and *SHELXTL*. Versions 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.