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3-(4-Fluorobenzyl)-2-thioxo-3,4,5,6-tetrahydropyrimidin-4(1*H*)-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.03 Å
R factor = 0.032
wR factor = 0.096
Data-to-parameter ratio = 13.8

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

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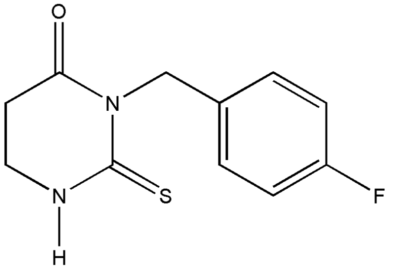
The tetrahydropyrimidine ring of the title molecule, $C_{11}H_{11}FN_2OS$, adopts a half-chair conformation. In the crystal structure, the molecules are linked to form centrosymmetric hydrogen-bonded dimers.

Comment

Derivatives of uracil and thiouracil are of interest because of their wide-ranging bioactivity (Gupta *et al.*, 2004; South *et al.*, 2003). For example, lenacil, bromacil, butafenacil, flupropacil, isocil and terbacilare are widely used as herbicides. Some derivatives also exhibit antidiabetic activity (Soliman, 1979). In addition, compounds that contain fluorine have special bioactivity; for example, flumioxazin is a widely used herbicide (Hermann *et al.*, 2003; Ulrich, 2004). This led us to study the synthesis and relationship between structure and herbicidal activity in a variety of fluorinated derivatives of uracil and thiouracil. We report here the crystal structure of the title compound, (I).



(I)

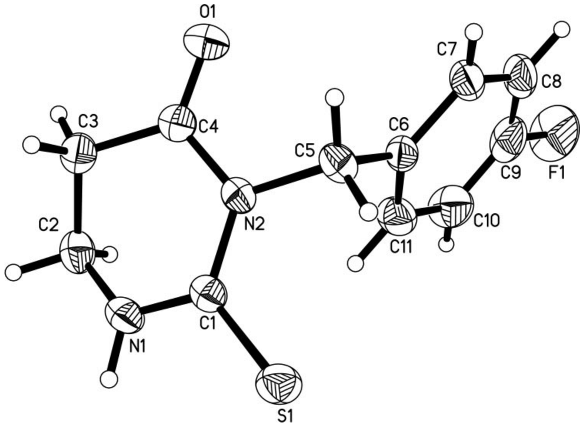


Figure 1
The structure of (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme. H atoms are drawn as spheres of arbitrary radius.

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The molecular structure of (I) is shown in Fig. 1. The tetrahydropyrimidine ring adopts a half-chair conformation, similar to that observed in related structures (Lorente & Aurrecoechea, 1994; Rohrer & Sundaralingam, 1968; Furberg & Jensen, 1968; Yao *et al.*, 2004*a*,*b*). The conformation of the attachment of the benzene ring to the tetrahydropyrimidine ring is described by the torsion angle C1—N2—C5—C6 of 103.52 (17)°. In the crystal structure, centrosymmetrically related molecules form dimeric pairs through intermolecular $\mathrm{N-H\cdots S}$ hydrogen bonds (Fig. 2 and Table 1).

Experimental

According to the reported procedure of Hatam *et al.* (1996), the title compound was synthesized by refluxing methyl 3-({[(4-fluorobenzyl)amino]carbonothioyl}amino)propanoate in triethylamine for about 2 h. After cooling, the precipitate was filtered off and recrystallized from a mixture of acetone and ethanol, giving single crystals suitable for X-ray diffraction.

Crystal data

$C_{11}H_{11}FN_2OS$
$M_r = 238.28$
Triclinic, $P\overline{1}$
$a = 6.392\ (3)$ Å
$b = 9.081\ (4)$ Å
$c = 11.099\ (5)$ Å
$\alpha = 113.793\ (6)^\circ$
$\beta = 95.328\ (7)^\circ$
$\gamma = 99.931\ (6)^\circ$
$V = 571.2\ (4)$ Å^3
$Z = 2$
$D_x = 1.385$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1012 reflections
$\theta = 3.3$–26.5°
$\mu = 0.28$ mm^{-1}
$T = 293\ (2)$ K
Prism, colorless
$0.22 \times 0.20 \times 0.18$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.772$, $T_{\max} = 1.000$
2984 measured reflections
2005 independent reflections
1725 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.014$
$\theta_{\max} = 25.0^\circ$
$h = -7 \rightarrow 6$
$k = -10 \rightarrow 8$
$l = -8 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.096$
$S = 1.07$
2005 reflections
145 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 0.1179P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.005$
$\Delta\rho_{\max} = 0.20$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

$D-\mathrm{H}\cdots A$	$D-\mathrm{H}$	$\mathrm{H}\cdots A$	$D\cdots A$	$D-\mathrm{H}\cdots A$
$\mathrm{N1-H1}A\cdots\mathrm{S1^{i}}$	0.90	2.71	3.4905 (18)	146
$\mathrm{N1-H1}A\cdots\mathrm{O1^{ii}}$	0.90	2.59	3.035 (2)	111

Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $1+x, y, z$.

H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å and N—H = 0.90 Å, and included in the final cycles of refinement using a riding model, with $U_{\rm iso}(\mathrm{H}) = 1.2U_{\rm eq}$(parent atom).

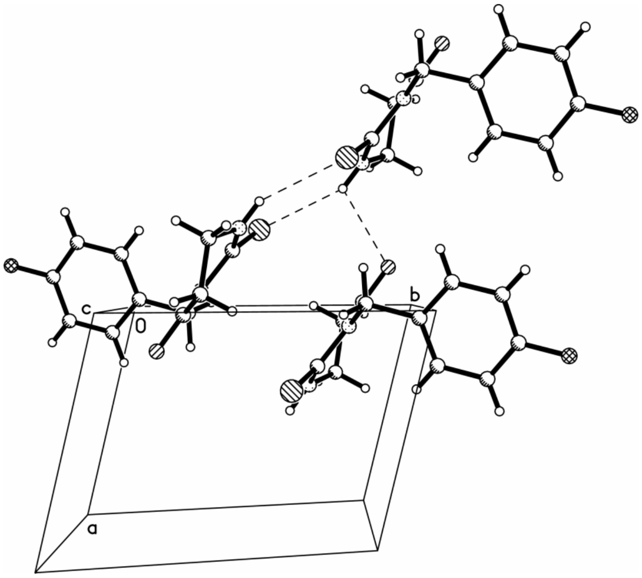

Figure 2
$\mathrm{N-H\cdots S}$ hydrogen-bonded dimers in (I), viewed down the *c* axis. Intermolecular hydrogen bonds are indicated by dashed lines.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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