

5-Acetyl-4-(4-methoxyphenyl)-6-methyl-3,4-dihydropyrimidine-2(1H)-thione

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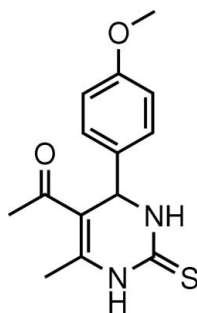
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Key indicators: single-crystal X-ray study; $T = 110$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.039; wR factor = 0.112; data-to-parameter ratio = 14.3.

In the title molecule, $\text{C}_{14}\text{H}_{16}\text{N}_2\text{O}_2\text{S}$, the heterocyclic ring adopts an envelope conformation with the plane through the five coplanar atoms making a dihedral angle of 88.99 (4) $^\circ$ with the benzene ring, which adopts an axial orientation. The thionyl, acetyl and methyl groups all have equatorial orientations. Intermolecular $\text{N}-\text{H}\cdots\text{S}$, $\text{N}-\text{H}\cdots\text{O}$, $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{S}$ hydrogen bonds are found in the crystal structure.

Related literature

For related crystal structures and their chemical and biological applications, see: Anuradha *et al.* (2008, 2009); Chitra *et al.* (2009).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{16}\text{N}_2\text{O}_2\text{S}$

$M_r = 276.36$

Monoclinic, $P2_1/n$
 $a = 12.0415$ (2) Å
 $b = 6.2219$ (1) Å
 $c = 18.0192$ (3) Å
 $\beta = 100.901$ (1) $^\circ$
 $V = 1325.66$ (4) Å³

$Z = 4$
Cu $K\alpha$ radiation
 $\mu = 2.17$ mm⁻¹
 $T = 110$ K
 $0.53 \times 0.13 \times 0.10$ mm

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis Pro*; Oxford Diffraction, 2009)
 $T_{\min} = 0.418$, $T_{\max} = 1.000$

5263 measured reflections
2616 independent reflections
2447 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.112$
 $S = 1.09$
2616 reflections
183 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.44$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.28$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{S2}^i$	0.87 (2)	2.61 (2)	3.464 (1)	169.3 (18)
$\text{N3}-\text{H3}\cdots\text{O14}^{ii}$	0.85 (2)	2.15 (2)	2.985 (2)	170 (2)
$\text{C16}-\text{H16B}\cdots\text{O15}^{iii}$	0.98	2.46	3.4377 (17)	176
$\text{C42}-\text{H42}\cdots\text{O15}^{iv}$	0.95	2.42	3.310 (2)	156
$\text{C61}-\text{H61B}\cdots\text{S2}^i$	0.98	2.80	3.7190 (14)	157

Symmetry codes: (i) $-x + 2, -y + 1, -z + 1$; (ii) $-x + 1, -y, -z + 1$; (iii) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $x, y + 1, z$.

Data collection: *CrysAlis Pro* (Oxford Diffraction, 2009); cell refinement: *CrysAlis Pro*; data reduction: *CrysAlis Pro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2363).

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