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Ethyl 4-(2-hydroxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

Cheng Qing-Fang,* Xing-You Xu, Jing-Yan Bao and Chun-Fang Zhang

Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China

Correspondence e-mail: cheng_qingfang@yahoo.com.cn

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In the title molecule, $C_{14}H_{16}N_2O_4$, all bond lengths and angles are normal. The crystal packing is stabilized by intermolecular O—H···O hydrogen bonds involving the hydroxy and keto groups, and by N—H···O hydrogen bonds involving the amino and keto groups.

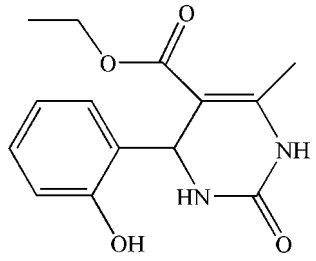
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.135
Data-to-parameter ratio = 12.8

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

Comment

As part of our study of 2-oxo-1,2,3,4-tetrahydropyrimidine derivatives, which demonstrate various pharmacological activities (Kappe *et al.*, 1999; Legeay *et al.*, 2007), we report here the structure of the title compound, (I).



(I)

In (I) (Fig. 1), all bond lengths and angles agree well with those reported for related compounds (Portilla *et al.*, 2006). The hydroxy and keto groups are involved in intermolecular O—H···O hydrogen bonds (Table 1), which link the molecules into zigzag chains running along the *c* axis. Weak intermolecular N—H···O hydrogen bonds (Table 1) further link two neighbouring chains with the formation of eight- and 16-membered rings (Fig. 2).

Experimental

A mixture of urea (51 mmol), ethyl acetoacetate (75 mmol) and salicylaldehyde (50 mmol) in absolute ethanol (30 ml) and concentrated hydrochloric acid (10 drops) was heated to reflux for 3 h. Upon cooling to room temperature, a crude product crystallized. The precipitate was filtered off and washed with propan-2-ol. The crude product was recrystallized from propan-2-ol to afford the desired product as a colourless solid (m.p. 490 K). Colourless single crystals of (I) were obtained by slow evaporation of an aqueous ethanol (90%) solution at ambient temperature after 7 d.

Crystal data

$C_{14}H_{16}N_2O_4$
M_r = 276.29
Monoclinic, $C2/c$
a = 20.757 (3) Å
b = 9.042 (2) Å
c = 13.919 (2) Å
β = 92.313 (3)°
V = 2610.2 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.32 × 0.16 × 0.13 mm

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Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.967, T_{max} = 0.987
6587 measured reflections
2308 independent reflections
1363 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.135
S = 1.03
2308 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	2.45	3.205 (5)	147
N2—H2···O3^{ii}	0.86	2.27	3.117 (4)	167
O4—H4···O3^{iii}	0.82	1.98	2.755 (4)	158

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

All H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, N—H = 0.86 Å and O—H = 0.82 Å, and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,N,O).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000) and *DIAMOND* (Brandenburg, 2004); software used to prepare material for publication: *SHELXTL*.

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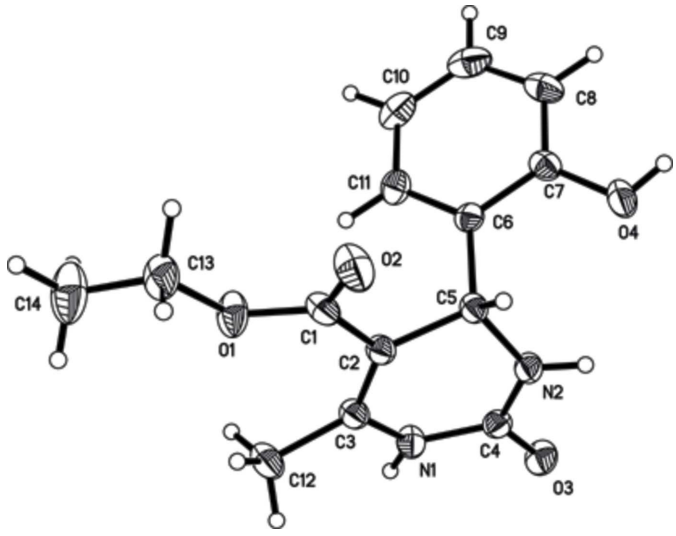

Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

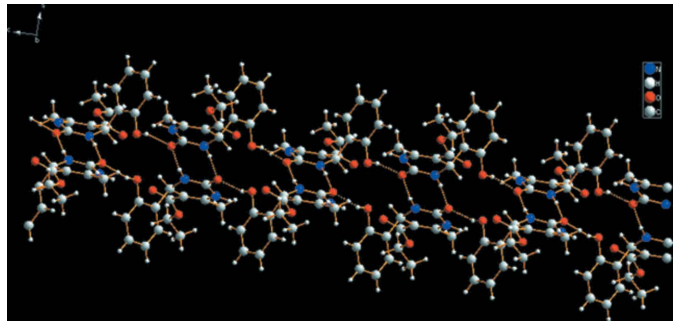

Figure 2
A portion of the crystal packing of (I), showing the intermolecular hydrogen bonds as dashed lines.

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