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3-(1*H*-Imidazol-1-yl)-1-(4-methoxyphenyl)-propan-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.124
Data-to-parameter ratio = 15.2

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

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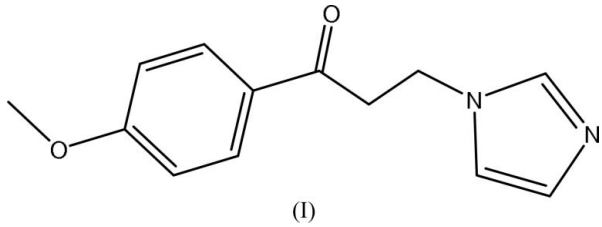
In the title compound, $C_{13}H_{14}N_2O_2$, molecules are linked into zigzag layers by intermolecular C—H···O and C—H···N hydrogen bonds. The packing is further stabilized by weak C—H···π interactions, forming a three-dimensional framework.

Comment

In the title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and compare well with those reported in a related compound (Wan *et al.*, 2005). The whole molecule is nearly planar, the largest deviation being 0.074 (1) Å for C11. However, the two aromatic rings are slightly twisted with respect to each other by a dihedral angle of 5.25 (9)°.



(I)

In the crystal structure, molecules are linked into zigzag layers by intermolecular C—H···O and C—H···N hydrogen bonds (Fig. 2 and Table 1). The packing is further stabilized by weak C—H···π interactions (Table 1), leading to a three-dimensional network.

Experimental

To a solution of 3-(dimethylamino)-1-(4-methoxyphenyl)propan-1-one (10.3 g, 0.05 mol) in water (25 ml) was added imidazole (4.4 g, 0.06 mol). The mixture was heated under reflux for 4 h, yielding a copious precipitate. Colorless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of an ethyl acetate–petroleum ether (1:1 *v*/*v*) solution over a period of two weeks.

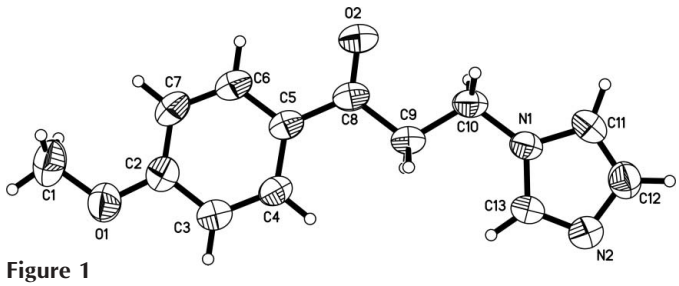


Figure 1
The structure of compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Crystal data

$C_{13}H_{14}N_2O_2$
M_r = 230.26
Monoclinic, $C2/c$
a = 21.349 (6) Å
b = 5.2657 (14) Å
c = 21.303 (6) Å
β = 97.600 (4)°
V = 2373.8 (11) Å^3
Z = 8
D_x = 1.289 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1951 reflections
θ = 2.5–24.7°
μ = 0.09 mm^{-1}
T = 293 (2) K
Needle, colorless
0.49 × 0.21 × 0.11 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (using intensity measurements) (*SADABS*; Sheldrick, 1996)
T_{min} = 0.958, T_{max} = 0.990
6335 measured reflections
2343 independent reflections
1855 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 26.1°
$h = -25 \rightarrow 26$
$k = -6 \rightarrow 6$
$l = -19 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.124
S = 1.02
2343 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0662P)^2 + 0.6137P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11A···O2^{i}	0.93	2.45	3.328 (2)	158
C13—H13A···N2^{ii}	0.93	2.50	3.418 (2)	170
C1—H1A···$Cg1^{iii}$	0.96	2.75	3.782	151
C1—H1B···$Cg2^{iv}$	0.97	2.78	3.622	146
C9—H9A···$Cg1^{iv}$	0.97	2.85	3.709	142
C9—H9B···$Cg2^{v}$	0.97	2.81	3.629	142

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

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with U_{iso}(H) = 1.2–1.5U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

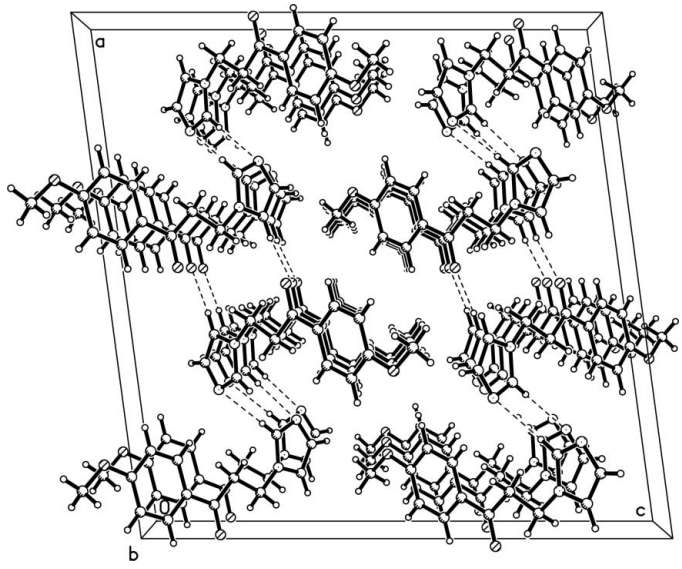


Figure 2
A view down the b axis. C—H···O and C—H···N hydrogen bonds are indicated by dashed lines.

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