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3-(1*H*-Imidazol-1-yl)-1-phenylpropan-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 = 0.122
Data-to-parameter ratio = 14.9

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

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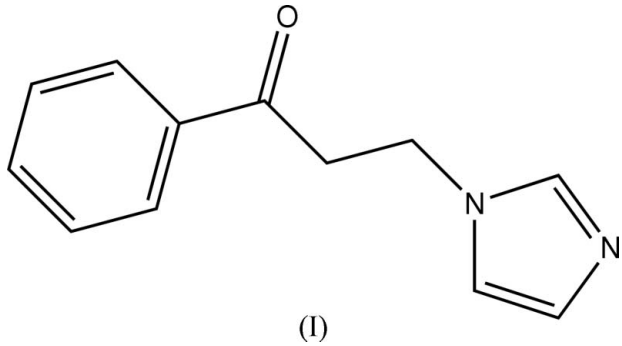
In the title compound, $C_{12}H_{12}N_2O$, the benzene and imidazole rings are almost perpendicular to each other, displaying a dihedral angle of 89.3 (1)°.

Comment

A view of the molecule of the title compound, (I), is shown in Fig. 1. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are comparable to those observed in a related compound (Wan *et al.*, 2005). The molecule of (I) is non-planar; the benzene and imidazole rings are almost perpendicular to each other, displaying a dihedral angle of 89.3 (1)°. The packing is stabilized by van der Waals interactions.



(I)

Experimental

To a solution of 3-(dimethylamino)-1-phenylpropan-1-one (10.35 g, 0.05 mol) in water (40 ml) was added imidazole (4.08 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 a dichloromethane–petroleum ether (1:1 *v*/*v*) solution over a period of 5 d.

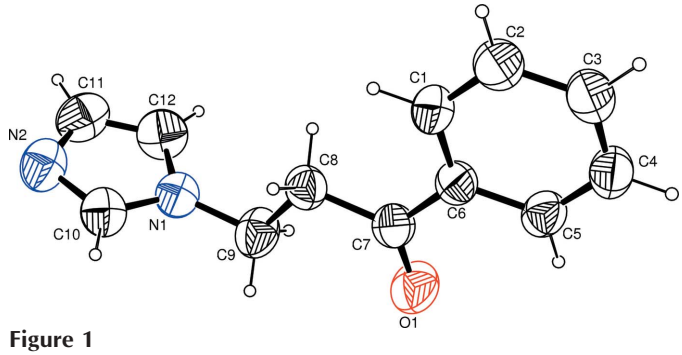


Figure 1
A view of the molecule of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. H atoms are shown as small spheres of arbitrary radii.

Crystal data

$C_{12}H_{12}N_2O$	D_x = 1.289 Mg m^{-3}
M_r = 200.24	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2368 reflections
a = 12.5860 (14) Å	θ = 2.6–25.7°
b = 10.3777 (12) Å	μ = 0.08 mm^{-1}
c = 8.0771 (9) Å	T = 293 (2) K
β = 102.095 (2)°	Block, colorless
V = 1031.6 (2) Å^3	0.48 × 0.21 × 0.17 mm
Z = 4	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	2028 independent reflections
ω scans	1748 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.018
T_{min} = 0.961, T_{max} = 0.984	θ_{max} = 26.0°
5671 measured reflections	$h = -15 \rightarrow 15$
	$k = -12 \rightarrow 12$
	$l = -9 \rightarrow 5$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0644P)^2 + 0.1568P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.122	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
2028 reflections	
136 parameters	
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

O1—C7	1.2152 (16)	C7—C8	1.5052 (19)
C6—C7	1.4960 (19)	C8—C9	1.514 (2)

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 $U_{iso}(H) = 1.2U_{eq}(C)$.

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: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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