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(1-Benzylpiperidin-4-ylidene)acetonitrile

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.065
wR factor = 0.158
Data-to-parameter ratio = 14.8

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

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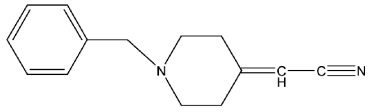
The title compound, $C_{14}H_{16}N_2$, crystallizes in a monoclinc unit cell. All bond lengths and angles are normal. The crystal structure is stabilized by van der Waals interactions.

Comment

In our studies, we have synthesized a series of acetylcholinesterase inhibitors such as 3-aminoalkyl-substituted pyridazines from 3-chloropyridazines and primary amines. The title compound, (I), is an intermediate in the formation of 2-(1-benzylpiperidin-4-yl)ethylamine, which possesses a lipophilic cationic head and helps enhance acetylcholinesterase inhibition (Wermuth *et al.*, 1989).



(I)

In (I) (Fig. 1), the piperidine ring has a chair conformation. The dihedral angles between the planes N1/C1/C5 and C1/C2/C4/C5, C2/C3/C4 and C1/C2/C4/C5, and C1/C2/C4/C5 and the benzene ring are 53.00 (2), 48.75 (3) and 87.82 (1)°, respectively. Atoms N1 and C3 deviate from the C1/C2/C4/C5 plane by 0.6671 (4) and −0.6168 (4) Å, respectively. C8 is displaced from the benzene ring plane and C1/C2/C4/C5 by −0.0357 (4) and 0.6469 (6) Å, respectively. Selected geometric parameters of (I) are listed in Table 1. The crystal structure is stabilized by van der Waals interactions.

Experimental

The title compound was synthesized according to Contreras *et al.* (1999). The crude product was purified by flash chromatography (EtOAc–hexane 1:1). The yield of product was 85% (m.p. 363 K). 1-Benzylpiperidin-4-ylideneacetonitrile (100 mg) was dissolved in EtOAc–hexane (2 ml). The solution was allowed to evaporate slowly over several days. Colorless crystals suitable for X-ray crystallography were collected when all of the solution had evaporated.

Crystal data

$C_{14}H_{16}N_2$
M_r = 212.29
Monoclinic, $P2_1/c$
a = 6.442 (2) Å
b = 15.681 (5) Å
c = 12.120 (4) Å
β = 94.579 (6)°
V = 1220.5 (7) Å^3
Z = 4
D_x = 1.155 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6062 reflections
θ = 3.2–19.1°
μ = 0.07 mm^{-1}
T = 298 (2) K
Block, colorless
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2142 independent reflections
ω scans	1128 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.057$
$T_{min} = 0.986$, $T_{max} = 0.993$	$\theta_{max} = 25.0^\circ$
5816 measured reflections	$h = -7 \rightarrow 7$
	$k = -14 \rightarrow 18$
	$l = -12 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 0.039P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.065$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.158$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -0.11$ e Å^{-3}
2142 reflections	
145 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

N1—C8	1.469 (3)	C3—C6	1.333 (3)
N2—C7	1.138 (4)	C6—C7	1.427 (4)
C9—C8	1.498 (3)		
C5—N1—C1	110.1 (2)	C6—C3—C4	122.8 (3)
C5—N1—C8	110.5 (2)	C2—C3—C4	112.8 (2)
N1—C8—C9	113.9 (2)	C3—C2—C1	109.6 (2)
N1—C5—C4	111.5 (2)	N1—C1—C2	111.5 (2)
C3—C4—C5	110.4 (2)	C3—C6—C7	122.3 (3)
C6—C3—C2	124.3 (3)	N2—C7—C6	179.8 (4)

H atoms were placed in calculated positions and allowed to ride on their parent atoms, with U_{iso}(H) values set at $1.5U_{eq}$(parent atom) for the Csp^3 H atoms and at $1.2U_{eq}$(parent atom) for the Csp^2 H atoms. The C—H distances were in the range 0.93–0.97 Å.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* and *SHELXTL* (Bruker, 2000); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

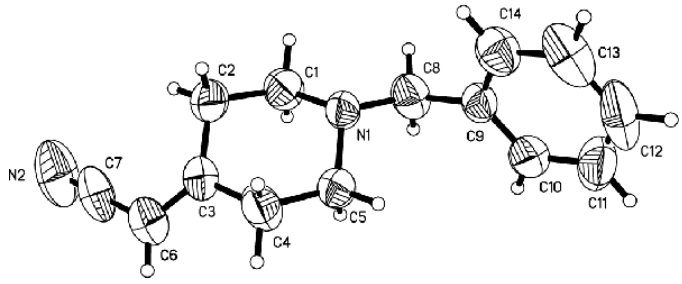


Figure 1
A view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

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