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N-Benzyl-*N*-(2-methoxyphenyl)cyclohex-1-enecarboxamide

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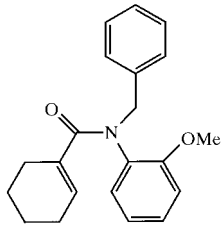
The title amide, $C_{21}H_{23}NO_2$, (I), does not photocyclize in the solid state. The methoxy group is involved in intermolecular steric interactions and so prevents the rotation of the *N*-phenyl group in the crystal.



(I)

Experimental

The title compound was prepared by one of the authors (HA) in a study on photocyclization of enamides and thioamides in the solid state (Aoyama, 2000). Crystals were grown from a hexane solution.

Crystal data

$C_{21}H_{23}NO_2$
M_r = 321.42
Monoclinic, $P2_1/n$
a = 10.485 (3) Å
b = 8.179 (1) Å
c = 20.985 (1) Å
β = 100.98 (1)°
V = 1766.7 (6) Å^3
Z = 4
D_x = 1.208 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 28.8–30.0°
μ = 0.609 mm^{-1}
T = 248 (1) K
Plate-like, colourless
0.50 × 0.50 × 0.05 mm

Data collection

Rigaku AFC-7*R* diffractometer
θ–2θ scans
Absorption correction: by integration (Coppens *et al.*, 1965)
T_{min} = 0.765, T_{max} = 0.969
4069 measured reflections
3388 independent reflections
2631 reflections with $I > 2\sigma(I)$
R_{int} = 0.010
θ_{max} = 75°
$h = 0 \rightarrow 13$
$k = -5 \rightarrow 10$
$l = -26 \rightarrow 26$
3 standard reflections
every 150 reflections
intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.055
$wR(F^2)$ = 0.159
S = 1.04
3388 reflections
217 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.0708P)^2 + 0.9854P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected geometric parameters (Å).

O1—C4	1.224 (2)	C6—C7	1.488 (4)
N3—C4	1.369 (3)	C7—C8	1.366 (5)
C4—C5	1.493 (3)	C8—C9	1.488 (4)
C5—C6	1.486 (3)	C9—C10	1.493 (4)
C5—C10	1.340 (3)		

X-ray intensity data were measured for $+h,+k,\pm l$ ($\theta < 75°$) and for $+h,-k,\pm l$ ($\theta < 30°$). The completeness of symmetry unique reflections ($\theta < 75°$) was 93.3%, which was due to the blind region of the low-temperature apparatus. All H-atom positional parameters were calculated geometrically and fixed with U_{iso}(H) = 1.2U_{eq}(parent atom). For the cyclohexene ring, the C5—C6 and C5═C10 axes were assigned to be single and double bonds, respectively, based on the bond lengths [1.486 (3) Å and 1.340 (3) Å, respectively]. The short C7—C8 bond length of 1.366 (5) Å may be an artifact due to the conformational disorder of the six-membered ring.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *TEXSAN*.

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