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N-(2-Naphthyloxymethylcarbonyl)pyrrolidine

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Key indicators

Single-crystal X-ray study
T = 160 K
Mean σ(C–C) = 0.002 Å
R factor = 0.052
wR factor = 0.144
Data-to-parameter ratio = 21.4

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

N-(2-Naphthyloxymethylcarbonyl)pyrrolidine, $C_{16}H_{17}NO_2$, is a potential antiamnesic agent. In the solid state, the pyrrolidine ring adopts an envelope conformation. Except for the atom of the envelope flap, the entire molecule is essentially planar.

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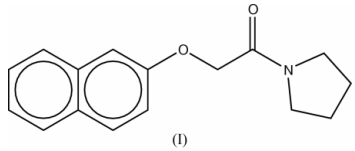
2-(2-Naphthyloxy)acetate derivatives, part IV.

Comment

The conformation of molecules with antiamnesic activity has attracted considerable interest (Amato *et al.*, 1991). The pyrrolidine moiety is a requisite for several active compounds currently used in the therapy of pathological brain-aging phenomena (Piracetam, Oxyracetam and Pramiracetam). The ring-extended *N*-analogues of 2-pyrrolidinone, *viz*. 2-aryl-3-piperazinone compounds, have been found to possess the characteristic nootropic pharmacological profile (Amato *et al.*, 1991). The present paper reports the structure and conformation of the title compound, (I), which was determined as a continuation of the investigation of a new class of antiamnesic agents (Thamotharan, Parthasarathi, Gupta *et al.*, 2003*a*,*b*,*c*; Thamotharan, Parthasarathi, Malik *et al.*, 2003*a*,*b*).



(I)

Fig. 1 shows a view of the molecule of (I), with the atomic numbering scheme. The bond lengths and angles in (I) are comparable with those in the related structures of 1-(2-naphthyloxymethylcarbonyl)piperidine and 3-methyl-1-(2-naphthyloxymethylcarbonyl)piperidine (Thamotharan, Parthasarathi, Malik *et al.*, 2003*a*), 4-(2-naphthyloxymethylcarbonyl)morpholine and 4-methyl-1-(2-naphthyloxymethylcarbonyl)piperazine (Thamotharan, Parthasarathi, Gupta *et al.*, 2003*a*), as well as *N*,*N*-dimethyl-2-(2-naphthyloxy)acetamide monohydrate (Thamotharan, Parthasarathi, Gupta *et al.*, 2003*c*). In (I), the central fragment C2—O11—C12—C13—N14 is planar, with a maximum deviation of 0.0223 (13) Å for atom C12. This central unit is virtually coplanar with the plane of the naphthalene moiety, the angle between the planes being 1.48 (5)°. The C2—O11—C12—C13 and O11—C12—C13—N14 torsion angles show that the central unit has an antiperiplanar conformation.

The pyrrolidine ring in nootropics usually has a half-chair (C_2, twist-envelope) conformation, (Thamotharan, Parthasarathi, Malik *et al.*, 2003*b* and references therein). In (I), however, the pyrrolidine ring adopts an envelope conforma-

tion, with atom C17 as the flap, a pseudo-rotation angle Δ = 86.0 (1)° and a maximum torsion angle φ_m = 36.5 (1)° (Rao *et al.*, 1981) for the atom sequence N14—C15—C16—C17—C18. Ignoring C17, the mean plane through the remainder of the pyrrolidine ring is almost coplanar with the plane of the naphthalene moiety, the angle between the planes being 3.55 (9)°. Thus, the entire molecule is essentially planar.

The exocyclic bond angle C1—C2—O11 deviates significantly from the normal value of 120° (Table 1) and this may be due to steric repulsion (H1···H121 = 2.31 Å, H1···H122 = 2.28 Å). The crystal packing is influenced only by normal van der Waals contacts.

Experimental

Methyl 2-(2-naphthyloxy)acetate (0.5 g) was reacted with pyrrolidine. The oily product obtained was treated with water. The precipitate obtained was filtered, dried and crystallized from acetone to afford (I) (yield, 0.51 g, 86.39%; m.p. 397–399 K).

Crystal data

$C_{16}H_{17}NO_2$	D_x = 1.343 Mg m^{-3}
M_r = 255.31	Mo Kα radiation
Monoclinic, $P2_1/c$	Cell parameters from 3899 reflections
a = 10.6427 (2) Å	θ = 2.0–30.0°
b = 8.8035 (2) Å	μ = 0.09 mm^{-1}
c = 14.4306 (2) Å	T = 160 (2) K
β = 110.9738 (11)°	Prism, colourless
V = 1262.46 (4) Å^3	0.23 × 0.20 × 0.17 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	R_{int} = 0.047
φ and ω scans with κ offsets	θ_{max} = 30.0°
Absorption correction: none	$h = 0 \rightarrow 14$
33348 measured reflections	$k = 0 \rightarrow 12$
3686 independent reflections	$l = -20 \rightarrow 18$
2775 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0765P)^2 + 0.209P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.052	
$wR(F^2)$ = 0.144	
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
3685 reflections	$\Delta\rho_{max}$ = 0.51 e Å^{-3}
172 parameters	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O11—C2—C1	125.64 (10)		
C2—O11—C12—C13	−178.34 (9)	O11—C12—C13—N14	178.81 (10)

All H atoms were placed in geometrically idealized positions (C—H = 0.95–0.99 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C). Reflection 1 0 0 was partially obscured by the beam stop and was omitted.

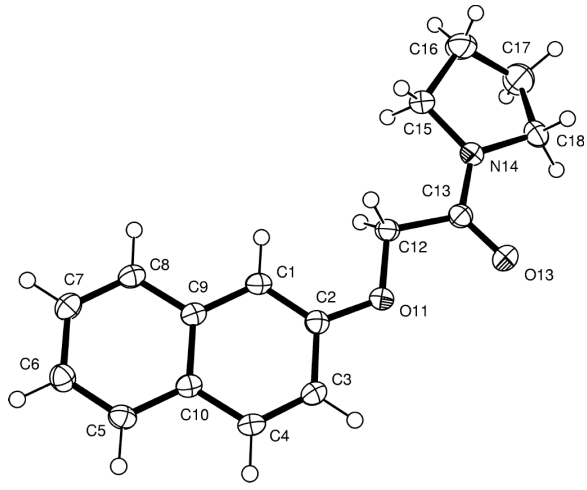


Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary radii.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2003).

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