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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.038
 wR factor = 0.093
Data-to-parameter ratio = 8.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.***tert*-Butyl 3-*endo*-3-hydroxy-8-azabicyclo-
[3.2.1]octane-8-carboxylate**

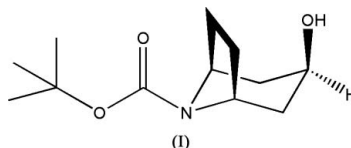
The title compound, $\text{C}_{12}\text{H}_{21}\text{NO}_3$, is an important intermediate for new dopamine transporter inhibitors. The six-membered ring of the azabicyclo[3.2.1]octane system adopts a chair conformation with the hydroxyl group axial. The fused five-membered ring is in an envelope conformation.

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Comment

A large number of azabicyclo[3.2.1]octane derivatives that bind at the cocaine binding site of the dopamine transporter (DAT) have been synthesized in order to better understand the pharmacological properties of this drug (Tamiz *et al.*, 2000). These compounds were also evaluated in radio-labelled binding assays for norepinephrine and serotonin transporters (Newman *et al.*, 1995). The title compound (I), an important intermediate in the preparation of new dopamine transporter inhibitors, was synthesized by the reaction of tropine and di-*tert*-butyl dicarbonate (Pedersen *et al.*, 2004) and its structure is reported here (Fig. 1).



The bond lengths and angles in the azabicyclo[3.2.1]octane fragment are in good agreement with those observed for a closely related structure, namely *endo*-3-[bis(4-fluorophenyl)methoxy]-8-methyl-8-azabicyclo[3.2.1]octane (Newman *et al.*, 1995). The six-membered ring adopts a chair conformation with the fused five-membered in an envelope conformation. The hydroxyl group is axial with the O1—C3—C2 and O1—C3—C4 angles 111.4 (2) and 108.5 (2)°, respectively. The dihedral angle between the two planes (defined by atoms C1/ C2/ C4/ C5 and C1/ C5/ C6/ C7) is 66.67 (10)°.

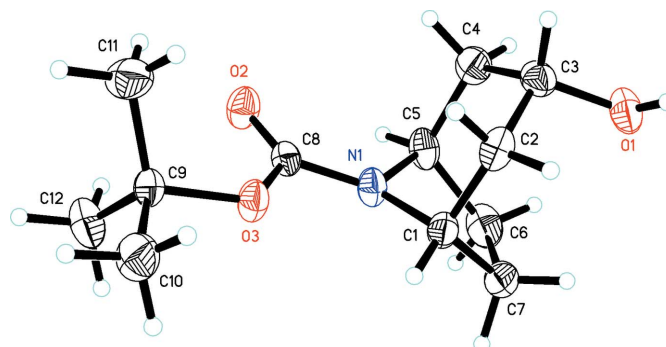


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Experimental

The title compound (I) was synthesized according to the method described previously by Pedersen *et al.* (2004) and identified by melting point, ¹H NMR, and ¹³C NMR. The crystal used for the data collection was obtained by slow evaporation of a saturated hexane-dichloromethane (**1:1 v/v**) [**OK?**] solution of (I) at room temperature.

Crystal data

C ₁₂ H ₂₁ NO ₃	Mo K α radiation
$M_r = 227.30$	Cell parameters from 2732 reflections
Orthorhombic, <i>Pna</i> 2 ₁	$\theta = 5.3\text{--}47.6^\circ$
$a = 11.1420$ (14) Å	$\mu = 0.09$ mm ⁻¹
$b = 10.4997$ (12) Å	$T = 293$ (2) K
$c = 10.7201$ (13) Å	Block, colorless
$V = 1254.1$ (3) Å ³	$0.50 \times 0.48 \times 0.30$ mm
$Z = 4$	
$D_x = 1.204$ Mg m ⁻³	

Data collection

Bruker SMART CCD area-detector diffractometer	1576 independent reflections
φ and ω scans	1353 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	$R_{\text{int}} = 0.080$
$T_{\text{min}} = 0.780$, $T_{\text{max}} = 1.000$	$\theta_{\text{max}} = 28.3^\circ$
7189 measured reflections	$h = -11 \rightarrow 14$
	$k = -13 \rightarrow 11$
	$l = -13 \rightarrow 14$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.038$	$w = 1/[\sigma^2(F_o^2) + (0.0605P)^2]$
$wR(F^2) = 0.093$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.94$	$(\Delta/\sigma)_{\text{max}} = 0.001$
1576 reflections	$\Delta\rho_{\text{max}} = 0.15$ e Å ⁻³
188 parameters	$\Delta\rho_{\text{min}} = -0.16$ e Å ⁻³

In the absence of significant anomalous dispersion effects, Friedel pairs were merged. The methyl H atoms were constrained to an ideal geometry (C–H = 0.96 Å), with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$, but were allowed to rotate freely about the C–C bonds. Other H atoms, located in a difference Fourier map, were refined freely. C–H distances are in the range 0.91 (2)–1.01 (3) Å and the O–H distance is 0.85 (4) Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1998); software used to prepare material for publication: *SHELXTL*.

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