The title compound, C_{14}H_{14}N_{2}O_{3}, was prepared by the base-catalyzed condensation reaction of 3-nitrobenzaldehyde with 1-azabicyclo[2.2.2]octan-3-one. The 3-nitrophenyl ring is twisted by 27.29 (19)° with respect to the plane of the C=C double bond connected to the azabicyclic ring. The molecule adopts the Z configuration.

Comment

In continuation of our work with 2-(substituted benzylidene/heteroaryl-3-ylmethylene)-1-azabicyclo[2.2.2]octan-3-ones (Sonar et al., 2004), as precursors of medicinal agents, we synthesized the title compound, (I). The compound was prepared by base-catalyzed condensation of 3-nitrobenzaldehyde with 1-azabicyclo[2.2.2]octan-3-one, to afford a single geometrical isomer. To study the structural conformation of the molecule, its X-ray crystal structure determination has been carried out.

In the title compound, the C1—C7 bond is in a trans disposition with respect to the C8—C9 bond and the molecule adopts the Z configuration. The C7—C8 double bond is nearly planar, as indicated by the value of 0.0091 (7) Å for the r.m.s. deviation of atoms N1, C8, C9, C7 and C1 from the mean plane passing through them. The Csp^2—N bond associated with the nitro group attached to the benzene ring is clearly of single-bond character [1.4739 (16) Å]. Deviations from the ideal...
afforded yellow needles of (I), which were suitable for X-ray analysis.
Spectroscopic analysis: $^1$H NMR (CDCl$_3$, δ, p.p.m.): 2.04–2.09 (td, 4H), 2.66–2.7 (p, 1H), 2.95–3.06 (m, 2H), 3.18–3.28 (m, 2H), 7.03 (s, 1H), 7.51–7.57 (t, 1H), 8.15–8.24 (m, 2H), 9.02–9.03 (t, 1H); $^1$C NMR (CDCl$_3$, δ, p.p.m.): 25.9, 40.4, 47.6, 122.3, 123.9, 126.6, 129.4, 135.6, 137.7, 146.9, 148.5, 205.7.

Crystal data

$C_{14}H_{14}N_2O_3$  
$M_r = 258.27$

Monoclinic. $P2_1/c$

$\alpha = 5.8905 (1) \AA$

$\beta = 24.2920 (4) \AA$

$\gamma = 8.5473 (2) \AA$

$\beta = 99.2211 (8)\text{o}$

$\nu = 1.1906 (4) \AA^3$

$Z = 4$

Data collection

Nonius KappaCCD area-detector diffractometer

$\omega$ scans

Absorption correction: multi-scan

(SCALEPACK; Otwinowski & Minor, 1997)

$T_{min} = 0.970, T_{max} = 0.980$

9090 measured reflections

Refinement

Refinement on $F^2$

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.099$

$S = 1.04$

2739 reflections

172 parameters

H-atom parameters constrained

Table 1

<table>
<thead>
<tr>
<th></th>
<th>$A$, θ (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1–C8</td>
<td>1.4448 (15)</td>
</tr>
<tr>
<td>N1–C12</td>
<td>1.4846 (15)</td>
</tr>
<tr>
<td>C1–C9</td>
<td>1.2223 (14)</td>
</tr>
<tr>
<td>C1–C7</td>
<td>1.4660 (16)</td>
</tr>
<tr>
<td>C2–C1–C7</td>
<td>123.18 (11)</td>
</tr>
<tr>
<td>O1–N2–C3</td>
<td>123.65 (11)</td>
</tr>
<tr>
<td>N2–C8–N1–C7</td>
<td>118.19 (11)</td>
</tr>
<tr>
<td>C6–C5–N2–C8</td>
<td>118.24 (11)</td>
</tr>
<tr>
<td>C2–C1–C7–C8</td>
<td>–154.52 (12)</td>
</tr>
<tr>
<td>C2–C1–C7–C8</td>
<td>27.29 (19)</td>
</tr>
</tbody>
</table>

H atoms were positioned geometrically and refined as riding, with C–H distances in the range 0.95–0.99 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: COLLECT (Nonius, 1999); cell refinement: SCALEPACK (Otwinowski & Minor, 1997); data reduction: DENZO-SMN (Otwinowski & Minor, 1997); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP in SHELXL/PC (Sheldrick, 1995); software used to prepare material for publication: SHELXL97 and local procedures.

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References
