(Z)-2-(2-Methylbenzylidene)-1-azabicyclo-[2.2.2]octan-3-one

The title compound, C_{15}H_{17}NO, has been synthesized by base-catalyzed condensation of 2-methylbenzaldehyde with 1-azabicyclo[2.2.2]octan-3-one and crystallization of the product with ethyl acetate. The geometry around the C=C bond is Z.

Comment

The title compound, (I), was prepared by base-catalyzed condensation of 2-methylbenzaldehyde with 1-azabicyclo[2.2.2]octan-3-one and the product was crystallized from ethyl acetate to afford a single geometrical isomer. The present X-ray crystallographic determination was carried out in order to determine both the geometry and the conformation of the molecule.

Fig. 1 shows a view of (I) and selected geometric parameters are presented in Table 1. The C1—C7 bond is in a trans disposition with respect to the C8—C13 bond. Deviations from ideal bond-angle geometry around the Csp^2 atoms of the double bonds are observed. The bond angles N9—C8—C13,
C7—C8—N9 and C8—C7—C1 (Table 1) are distorted because of the steric hindrance of the double bond linking the 2-methylphenyl ring with the azabicyclic moiety. These deviations significantly contribute to the relief of the intramolecular non-bonded interactions present in this portion of the molecule. The C6—C1—C7—C8 torsion angle indicates the deviation of the double bond from the plane of the benzene ring. However, the C1—C7 bond length suggests conjugation of the C7=C8 bond with electrons of the 2-methylphenyl ring (Wilson, 1992).

**Experimental**

The title compound was prepared according to the previously reported procedure of Sonar et al. (2003). Crystallization from ethyl acetate afforded yellow crystals.

**Crystal data**

\[ C_{15}H_{17}NO \]

\[ M_r = 227.30 \]

Monoclinic, \( P_2_1 \)

\[ a = 6.6514 (1) \text{ Å} \]

\[ b = 22.3378 (5) \text{ Å} \]

\[ c = 8.0734 (2) \text{ Å} \]

\[ \beta = 101.6068 (10) ^\circ \]

\[ V = 1175.00 (4) \text{ Å}^3 \]

**Data collection**

Nonius KappaCCD diffractometer

\( \omega \) scans

Absorption correction: multi-scan (SCALEPACK; Otwinowski & Minor, 1997)

\[ T_{\text{min}} = 0.975, \quad T_{\text{max}} = 0.978 \]

4984 measured reflections

2688 independent reflections

\[ wR_F = 0.057 \]

\[ S = 1.04 \]

2688 reflections

155 parameters

H-atom parameters constrained

\[ w = 1/[σ^2(F_o^2) + (0.0533P)^2 + 0.2705P] \]

where \( P = (F_o^2 + 2F_c^2)/3 \)

\( \Delta p_{\text{max}} = 0.28 \text{ e Å}^{-3} \)

\( \Delta p_{\text{min}} = -0.20 \text{ e Å}^{-3} \)

**Refinement**

\[ R(F^2) = 0.039 \]

\[ wR(F^2) = 0.107 \]

\[ S = 1.04 \]

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**Selected geometric parameters (Å, \(^\circ\)).**

<table>
<thead>
<tr>
<th>Bond/Angle</th>
<th>C1—C7</th>
<th>C8—C13</th>
<th>C1—C7</th>
<th>C8—C13</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1—C7</td>
<td>1.4678 (16)</td>
<td>1.4966 (16)</td>
<td>1.5029 (16)</td>
<td>1.4826 (15)</td>
</tr>
<tr>
<td>C2—C16</td>
<td>1.3744 (16)</td>
<td>1.2194 (14)</td>
<td>1.3744 (16)</td>
<td>1.2194 (14)</td>
</tr>
<tr>
<td>C7—C8</td>
<td>1.4427 (14)</td>
<td>1.4242 (14)</td>
<td>1.4427 (14)</td>
<td>1.4242 (14)</td>
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<tr>
<td>C8—N9</td>
<td>1.4121 (14)</td>
<td>1.4121 (14)</td>
<td>1.4121 (14)</td>
<td>1.4121 (14)</td>
</tr>
<tr>
<td>C1—C2—C16</td>
<td>121.44 (10)</td>
<td>121.44 (10)</td>
<td>121.44 (10)</td>
<td>121.44 (10)</td>
</tr>
<tr>
<td>C7—C8—C13</td>
<td>127.53 (11)</td>
<td>127.53 (11)</td>
<td>127.53 (11)</td>
<td>127.53 (11)</td>
</tr>
<tr>
<td>C7—C8—N9</td>
<td>124.50 (10)</td>
<td>124.50 (10)</td>
<td>124.50 (10)</td>
<td>124.50 (10)</td>
</tr>
<tr>
<td>C7—C8—C13</td>
<td>121.91 (11)</td>
<td>121.91 (11)</td>
<td>121.91 (11)</td>
<td>121.91 (11)</td>
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<tr>
<td>N9—C8—C13</td>
<td>113.53 (10)</td>
<td>113.53 (10)</td>
<td>113.53 (10)</td>
<td>113.53 (10)</td>
</tr>
<tr>
<td>C6—C1—C7—C8</td>
<td>34.30 (18)</td>
<td>34.30 (18)</td>
<td>34.30 (18)</td>
<td>34.30 (18)</td>
</tr>
<tr>
<td>C1—C7—C8—C13</td>
<td>177.27 (10)</td>
<td>177.27 (10)</td>
<td>177.27 (10)</td>
<td>177.27 (10)</td>
</tr>
</tbody>
</table>

H atoms were found in difference Fourier maps and subsequently placed in idealized positions with constrained C—H distances of 1.00 Å (R3CH), 0.99 Å (R2CH2), 0.98 Å (RCH3) and 0.95 Å (Csp2). \( U_{\text{iso}}(H) \) values were set to either 1.5 \( U_{\text{eq}} \) of the attached C atom (CH3) or 1.2 \( U_{\text{eq}} \) for all other H atoms.

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**References**