In the title compound, C_{19}H_{12}FNO, the dihedral angle between the mean planes of the 9H-xanthene moiety and the 3-fluorophenyl group is 82.5(1)^\circ. An intramolecular C—H⋯π interaction stabilizes the molecular conformation.

Comment

Molecular organization and molecular interactions are the features that are responsible for molecules exhibiting different functional properties. An understanding of non-covalent interactions becomes essential for interpreting and predicting relationships between chemical structure and function (Hunter et al., 2001). Crystal engineering, via manipulation of hydrogen bonding, has attracted a lot of interest in the recent literature (Aakeroy, 1997; Desiraju, 2000). Weak intermolecular forces of the type C—H⋯π play an important role in various systems of biological and chemical interest (Nishio, 2004). Intramolecular C—H⋯π interactions are responsible for molecules adopting a particular conformation in the solid state (Jennings et al., 2001). A structural study of the title compound, (I), has been carried out as a case study where there is no possibility of formation of hydrogen bonds and hence it is thought to be suitable for the study of weak interactions.

A view of (I) with the atom-labelling scheme is shown in Fig. 1. The 9H-xanthene unit is almost planar, as indicated by the torsion angles (Table 1). The bond angle C_{12}—N_{1}—C_{14} of 126.7(2)^\circ is greater than the ideal bond angle value of 120^\circ to avoid steric repulsion between atoms H_{15} and H_{1}. Rotation of the 3-fluorophenyl group takes place and this is favoured because it leads to the formation of an intramolecular C—H⋯π interaction (Table 2) involving H_{1}, which stabilizes the molecular conformation (Fig. 1).
H bond distances are in the range 0.89 (3)-1.08 (2) Å.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SIR2004 (Altomare et al., 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and CAMERON (Watkin et al., 1995); software used to prepare material for publication: PLATON (Spek, 2003).

We thank the Department of Science and Technology, India, for data collection on the CCD facility set up under the IRFA-DST program. D. Chopra thanks CSIR, India, for a Junior Research Fellowship.

References

Experimental
Compound (I) was synthesized according to a procedure reported in the literature (Nagarajan et al., 1974). The compound was crystallized from a solution in ethyl acetate and hexane, by slow evaporation at ca. 278 K.

Crystal data
C13H12FNO
M. = 289.30
Monoclinic. P21/n
a = 14.175 (3) Å
b = 5.0634 (9) Å
c = 19.912 (3) Å
β = 102.794 (4)°
V = 1393.6 (4) Å³
Z = 4

Crystallography Laboratory, University of Giittingen, Germany.

Data collection
Bruker SMART CCD area-detector diffractometer
ω and ω scans
Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)
Tmax = 0.902, Tmin = 0.949
10501 measured reflections

Refinement
Refinement on F²
wR² (F²) = 0.082
S = 1.12
2849 reflections
247 parameters
All H-atom parameters refined

Table 1
Selected geometric parameters (Å, °).

<table>
<thead>
<tr>
<th>Bond/Angle</th>
<th>Value (Å/°)</th>
</tr>
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<tbody>
<tr>
<td>N1—C12—N1—C14</td>
<td>1.28 (3)</td>
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<td>N1—C14—N1—C12</td>
<td>1.40 (4)</td>
</tr>
<tr>
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<td>126.7 (2)</td>
</tr>
<tr>
<td>C14—N1—C12—C13</td>
<td>-6.1 (5)</td>
</tr>
<tr>
<td>N1—C12—C11—C10</td>
<td>14 (4)</td>
</tr>
<tr>
<td>N1—C12—C13—C1</td>
<td>-5.8 (5)</td>
</tr>
<tr>
<td>C5—O1—C6—C7</td>
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Table 2
Hydrogen-bonding geometry (Å, °).

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<td>D—H···A'</td>
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Cg1 is the centroid of the C14—C19 ring.

All H atoms were located in difference Fourier maps and refined isotropically. The C—H bond distances are in the range 0.89 (3)-1.08 (2) Å.

Crystallography Laboratory, University of Giittingen, Germany.

Figure 1
The molecular structure of (I), showing 40% probability ellipsoids. H atoms have been omitted for clarity, except for H1. The dashed line indicates the intramolecular C—H···π interaction.

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