**1-(10,11-Dihydrodibenz[bf]azepin-5-yl)ethanone**

The asymmetric unit of the title compound, C_{16}H_{15}NO, comprises two independent molecules (A and B), both adopting a half-boat conformation, or butterfly shape. The intramolecular dihedral angles between the benzene rings in A and B are 64.40 (4) and 65.24 (5)°, respectively.

**Comment**

The title compound, (I), is used as an intermediate for the synthesis of carbamazepine and oxcarbazepine (Kricka & Ledwith, 1974), two anticonvulsant drugs whose structures have been reported [Grzesiak et al., 2003 (most recent form); Hempel et al., 2005]. As part of a series of studies into the structural aspects of iminostilbene analogues, the structure of (I) was determined and is reported here. A search of the Cambridge Structural Database (November 2004 version; Allen, 2002) reveals that there are 27 compounds reported that contain a 10,11-dihydrodibenz[b,f]azepine moiety with only two containing an additional N-acetyl group, viz. the N-acetyldibenz[b,f]azepine dimer (Harding, 1983) and its hydrate structure (Taga et al., 1986). The structure of (I) (Fig. 1) comprises two independent molecules, A and B, in the asymmetric unit, both of which adopt a half-boat conformation (Cremer & Pople, 1975) or butterfly shape. The intramolecular dihedral angles between the benzene rings in A and B are 64.40 (4) and 65.24 (5)°, respectively.

**Experimental**

The title compound was prepared by refluxing 10,11-dihydro-5H-dibenz[b,f]azepine (1.95 g, 10 mmol) in acetic anhydride (5 ml) for 6 h. Crystals were grown from methanol.

**Crystal data**

C_{16}H_{15}NO  
*M* = 237.29  
Orthorhombic, *P*2₁2₁2₁  
*a* = 9.5674 (2) Å  
*b* = 11.7020 (3) Å  
*c* = 22.2785 (4) Å  
*V* = 2494.25 (9) Å³  
*Z* = 8  
*D*ₐ = 1.264 Mg m⁻³  
Mo *Kα* radiation  
Cell parameters from 3179 reflections  
θ = 2.9–27.5°  
μ = 0.08 mm⁻¹  
*T* = 150 (2) K  
Prism, colourless  
0.60 × 0.40 × 0.10 mm

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Basavegowda Nagaraj et al.  
C_{16}H_{15}NO  
o1609
Data collection
Nonius KappaCCD diffractometer
\( \varphi \) and \( \omega \) scans
Absorption correction: multi-scan
(SADABS; Sheldrick, 2003)
\( T_{\text{max}} = 0.954, T_{\text{min}} = 0.992 \)
19122 measured reflections
2778 independent reflections
2540 reflections with \( I > 2\sigma(I) \)
\( R_{\text{int}} = 0.037 \)
\( \theta_{\text{max}} = 26.0^\circ \)
\( h = -11 \rightarrow 11 \)
\( k = -14 \rightarrow 14 \)
\( l = -27 \rightarrow 27 \)

Refinement
Refinement on \( F^2 \)
\( R[F^2 > 2\sigma(F^2)] = 0.031 \)
\( wR(F^2) = 0.076 \)
\( S = 1.02 \)
2778 reflections
328 parameters
H-atom parameters constrained
Extinction correction: SHELXL97
Extinction coefficient: 0.0285 (14)

All H atoms were included in the refinement at calculated positions, in the riding-model approximation, with C–H distances of 0.95 (ArH), 0.98 (CH\(_2\)) and 0.99 Å (CH\(_3\)). The isotropic displacement parameters for all H atoms were set equal to 1.25\( U_{eq} \) of the carrier atom. The absolute configuration could not be accurately determined from the diffraction data, thus 1600 Friedel opposites were merged and the configuration arbitrarily assigned. The number of Friedel pairs is 1660.

Data collection: COLLECT (Hooft, 1998); cell refinement: DENZO (Otwinowski & Minor, 1997) and COLLECT; data reduction: DENZO and COLLECT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

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References