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10-Methyl-9,11-annulated dibenzobarrelene

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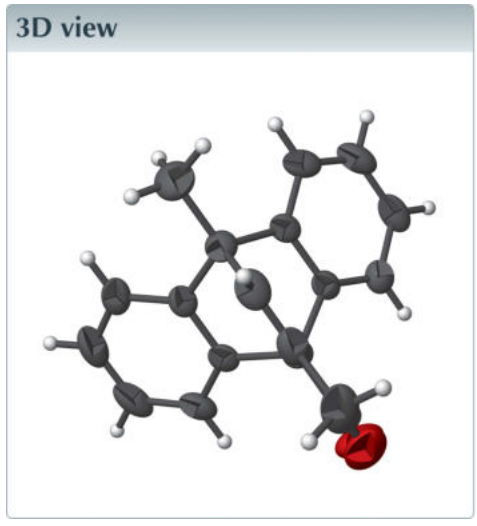
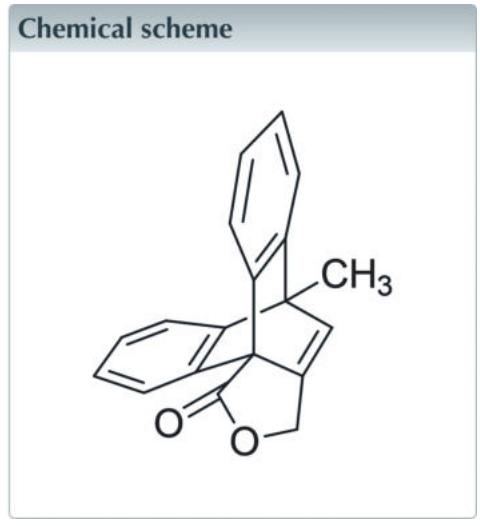
In the title compound (systematic name: 8-methyl-16-oxapentacyclo-[6.6.5.0^{1,18}.0^{2,7}.0^{9,14}]nonadeca-2,4,6,9(14),10,12,18-heptaen-15-one), $C_{19}H_{14}O_2$, the benzene rings form a dihedral angle of 64.84 (7)°. In the crystal, π–π stacking interactions, with a centroid–centroid distance of 3.7695 (8) Å, and weak C—H$\cdots\pi$ interactions link molecules along the *b*-axis direction.





Structure description

Dibenzobarrelene systems have attracted interest over the years because of their biological (Khalil *et al.*, 2010) and photochemical properties (Zimmerman & Grunewald, 1966). Suitably substituted dibenzobarrelenes exhibit interesting physical properties (Ishii *et al.*, 2016). Mathew *et al.* (2013, 2014) reported two dibenzobarrelene derivatives and discussed their structural features. A recent report highlighted the applications of dibenzobarrelenes in OLEDs and photoluminescent materials (Ishii *et al.*, 2018).

In the present study, an intramolecular Diels–Alder reaction was employed for the synthesis of 9,11-annulated dibenzobarrelenes and their diffraction-quality single crystals could be obtained by crystallization from suitable solvents. The derivatives can be easily modified structurally by using different substituents on the bridgehead positions. In the case of the title compound, the bridgehead position 10 is substituted with a methyl group and we obtained good-quality single crystals by recrystallization from acetonitrile. The molecular structure of the title compound is shown in Fig. 1. The two benzene rings form a dihedral of 64.84 (7)°. These rings form angles of 58.86 (8) and 56.96 (6)°, respectively, with the annulated ring at the vinyllic bridge head position.

In the crystal, π–π stacking interactions are present between inversion-related rings (C1–C4/C18/C19) with a centroid–centroid distance of 3.7695 (8) Å. Pairs of weak C—