A P212121 polymorph of (+)-clusianone

ABSTRACT

The title compound, C33H42O4[systematic name: (1S,5S,7R)-3-benzoyl-4-hydroxy-8,8-dimethyl-1,5,7-tris(3-methylbut-2-enyl) bicyclo[3.3.1]nona-3-ene-2,9-dione], has a central bicyclo[3.3.1]nonane-2,4,9- trione surrounded by tetraprenylated and benzoyl groups. The compound was recrystallized several times in methanol using both a slow evaporation method and with a crystal-seeding technique. This subsequently produced diffraction-quality crystals which crystallize in the orthorhombic space group P212121, in contrast to a previous report of a structure determination in the Pna21 space group [McCandlish et al. (1976). Acta Cryst. B32, 1793-1801]. The title compound has a melting point of 365-366 K, and a specific rotation [α]20value of +51.94°. A strong intramolecular O-H···O hydrogen bond is noted. In the crystal, molecules are assembled in the ab plane by weak C-H···O interactions.

Keyword: Single-crystal X-ray study; Clusianone.