Crystal structure and Hirshfeld surface analysis of a conformationally unsymmetrical bischalcone: (1E,4E)-1,5-bis(4-bromophenyl)penta-1,4-dien-3-one

ABSTRACT

In the title bischalcone, C17H12Br2O, the olefinic double bonds are almost coplanar with their attached 4-bromophenyl rings [torsion angles = 10.2 (4) and 6.2 (4)], while the carbonyl double bond is in an s-trans conformation with with respect to one of the C C bonds and an s-cis conformation with respect to the other [C C—C O = 160.7 (3) and 15.2 (4) , respectively]. The dihedral angle between the 4-bromophenyl rings is 51.56 (2) . In the crystal, molecules are linked into a zigzag chain propagating along [001] by weak C— H interactions. The conformations of related bischalcones are surveyed and a Hirshfeld surface analysis is used to investigate and quantify the intermolecular contacts.

Keyword: Crystal structure; Bischalcone; Pentadienone bridge; C—H interactions; Hirshfeld surface analysis