S-Benzyl 3-[1-(6-methylpyridin-2-yl)ethylidene]- dithiocarbazate: crystal structure and Hirshfeld surface analysis

ABSTRACT

In the title dithiocarbazate ester, C 16 H 17 N 3 S 2 (systematic name: (Z)-{[(benzylsulfanyl)methanethioyl]amino}[1-(6-methylpyridin-2-yl)ethylidene]amine), the central methylidenehydrazinecarbodithioate (C 2 N 2 S 2) core is almost planar (r.m.s. deviation = 0.0111 Å) and forms dihedral angles of 71.67 (3)° with the approximately orthogonally inclined thioester phenyl ring, and 7.16 (7)° with the approximately coplanar substituted pyridyl ring. The latter arrangement and the Z configuration about the imine-C=N bond allows for the formation of an intramolecular hydrazine-N—H...N(pyridyl) hydrogen bond that closes an S (6) loop. In the crystal, phenyl-C—H...S(thione), methylene-C—H...π(pyridyl), methylene- and phenyl-C—H...π(phenyl) contacts connect molecules into supramolecular layers propagating in the bc plane; the layers stack along the a axis with no directional interactions between them. The analysis of the Hirshfeld surface indicates the relative importance of an intralayer phenyl-H...H(pyridyl) contact upon the molecular packing.

Keyword: Crystal structure; Di-thio-carbazate ester; Hydrogen bonding; Hirshfeld surface analysis.