Benzyl N-[(Z)-(1-methyl-2-sulfanylpropylidene)amino]carbamodithioate.

ABSTRACT

The title compound, C12H16N2S3, was obtained by the condensation reaction of S-benzyl dithiocarbazate and 3-mercaptobutan-2-one. The phenyl ring and thiol (SH) group are approximately perpendicular [S—C—C—C and N—C—C—S torsion angles = 67.8 (3) and 116.9 (2)°, respectively] to the rest of the molecule. In the crystal, molecules are linked by weak S—H(...)S and N—H(...)S hydrogen bonds, π – π interactions between the benzene rings [centroid–centroid distance = 3.823 (2) Å] and C—H(...) π interactions.

Keyword: Single-crystal X-ray study; Data-to-parameter ratio = 16.9; R factor = 0.044.