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Title: Solid-phase synthesis and crystal structure of 5(3-nitrophenyl)-3,7-diphenyl-4H,6H-1,2-diazepine

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Abstract

The title compound, 5-(3-nitrophenyl)-3,7-diphenyl-4H,6H-1,2-diazepine (C₂₃H₁₉N₃O₂), was synthesized, in 76% yield, by one-pot multicomponent solid-phase reaction of 3-nitrobenzylidene phenyl ketone, acetophenone and hydrazine, using the catalyst bismuth nitrate, co-catalyst ZnCl₂, adsorbed on neutral alumina, at 110°C. The compound was characterized by spectral methods and X-ray diffraction studies. The crystals are monoclinic, space group *P2₁/c*: *a* = 12.186(2), *b* = 14.769(3), *c* = 11.046(2) Å, β = 115.023(3)°, *Z* = 4; *R* = 0.0418 for 2576 observed reflections. The diazepine ring assumes a twist chair conformation. The dihedral angles between the mean planes through the diazepine ring and the nitrophenyl rings and two phenyl are: 89.19(5)°, 45.85(5)° and 20.80(6)°, respectively. The crystal structure is stabilized by C-H...N, C-H...O, C-H...π hydrogen bonds and π-π-stacking interactions.

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