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Title: Synthesis and X-Ray Crystallographic Analysis of 2-(2, 4-Dimethyl Pyrrolyl) Benzothiazole

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Abstract

Synthesis of 2- (2, 4-dimethyl pyrrolyl) benzothiazole by chemical means and molecular structure by X-ray crystallographic techniques is reported. The compound crystallizes in the orthorhombic crystal system with space group Pbca and unit cell parameters: a = 12.161(9), b = 0.787(1),c = 16.792(2) Å, V = 2202.8(4) Å^3 and Z = 8. The final reliability index is 0.073 for 7,959 observed reflections. The benzothiazole and pyrrole rings exist in planar conformations. The dihedral angle between the least-squares planes of both these moieties is 13.31°. There exists an isolated C4–H4···N1 intermolecular interaction, besides two C–H···S and C–H···N intermolecular interactions. The presence of C–H···S and C–H···N intramolecular interactions make the present molecule look like a virtual two-six-membered and three-five-membered ring structure.

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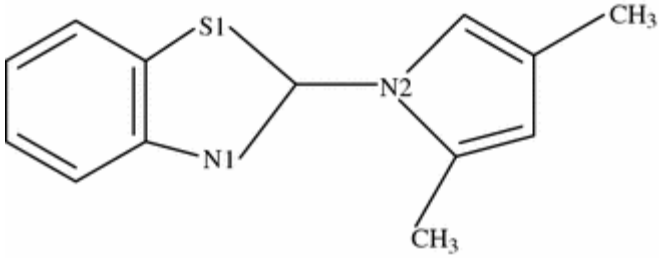
Chemical structure of 2-(2, 4-dimethyl pyrrolyl) benzothiazole



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