Synthesis, spectral and X-ray crystal structure of 3-(3-methoxyphenyl)-5-(3-methylthiophen-2-yl)-4,5-dihydro-1H-pyrazole-1-carboxamide: Hirshfeld surface, DFT calculations and thermo-optical studies

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PII: S2405-8300(17)30180-5
DOI: 10.1016/j.cdc.2018.01.001
Reference: CDC 90

To appear in: *Chemical Data Collections*

Received date: 15 December 2017
Revised date: 13 January 2018
Accepted date: 24 January 2018

Please cite this article as: Karthik Kumara , A. Dileep Kumar , K. Ajay kumar , N.K. Lokanath , Synthesis, spectral and X-ray crystal structure of 3-(3-methoxyphenyl)-5-(3-methylthiophen-2-yl)-4,5-dihydro-1H-pyrazole-1-carboxamide: Hirshfeld surface, DFT calculations and thermo-optical studies, *Chemical Data Collections* (2018), doi: 10.1016/j.cdc.2018.01.001

Synthesis, spectral and X-ray crystal structure of 3-(3-methoxyphenyl)-5-(3-methylthiophen-2-yl)-4,5-dihydro-1H-pyrazole-1-carboxamide: Hirshfeld surface, DFT calculations and thermo-optical studies

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Abstract: Novel pyrazole derivative, 3-(3-methoxyphenyl)-5-(3-methylthiophen-2-yl)-4,5-dihydro-1H-pyrazole-1-carboxamide was synthesized, characterized by NMR, mass spectra, FT-IR, UV-Visible, TG-DTG and finally the three dimensional structure was confirmed by single crystal X-ray diffraction studies. A dihedral angle of 78.51(13)° between the pyrazole and the thiophene rings confirms the twisted conformation between the rings. C—H···O and N—H···O hydrogen bond interactions are extended through 3D network to form $R_2^2(8)$ supramolecular motif. The compound was found to be thermally stable up to 190°C. Further, the intermolecular interactions of the crystal structure were analysed by Hirshfeld surface analysis. The molecular geometries and electronic structures of the compound were optimized, calculated with ab-initio methods. The electrophilic and nucleophilic regions of the molecular surface were identified. The solvent effects on the structural parameters were studied using different solvents. Non-linear optical properties of the title compound were investigated.

Keywords: 3+2 cycloaddition, pyrazole, X-ray diffraction, $R_2^2(8)$ ring motif, Hirshfeld surface.

Specifications Table

Subject area	Chemical Physics
Compound	**3-(3-methoxyphenyl)-5-(3-methylthiophen-2-yl)-4,5-dihydro-1H-pyrazole-1-carboxamide**
Data category	Synthesis, NMR (^{1}H and ^{13}C), mass spectra, FT-IR, crystallographic data and density functional theory calculations.
Data acquisition format	CIF for crystallography
Data type	Analyzed