m13.p20

C - H•••F, N / C - H•••S and C - H•••π interactions in 5-fluoro-1*H*-indole-2,3-dione-3-thiosemicarbazones

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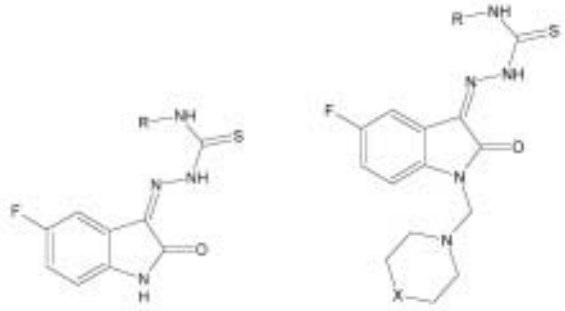
1*H*-Indole-2,3-dione is a versalite lead molecule for designing potential antiviral agents. Several authors found that 1*H*-indole-2,3-dione-3-thiosemicarbazone and its N-Mannich bases were active against various viruses. The first clinically approved antiviral agent, 1-methyl-1*H*-indole-2,3-dione-3-thiosemicarbazone (methisazone) and 1*H*-indole-2,3-dione-3-thiosemicarbazone are active against poxviruses. 1-Methyl-1*H*-indole-2,3-dione-3-(N,N-diethylthiosemicarbazone) and 1-allyl-1*H*-indole-2,3-dione-3-(N,N-diallylthiosemicarbazone) are effective compounds against HIV as reverse transcriptase inhibitors. In view of these observations, 5-fluoro-1*H*-indole-2,3-dione-3-thiosemicarbazones (**1**) obtained by condensation of 5-fluoro-1*H*-indole-2,3-dione with N-substituted-thiosemicarbazides were treated with morpholine or piperidine and formaldehyde to yield 1-morpholino/piperidinomethyl-5-fluoro-1*H*-indole-2,3-dione-3-thiosemicarbazones (**2**). The crystal and molecular structures of six derivatives of 5-fluoro-1*H*-indole-2,3-dione-3-thiosemicarbazones have been determined by X-ray analysis. The crystal packing of all compounds are governed by C - H•••F, N / C - H•••S and N / C - H•••π interactions. The approximate planarity of indole-thiosemicarbazone system is due to intramolecular hydrogen bonds existing in molecules.



m13.p21

N,N-Bis(2-hdroxybenzylidene) phenylen-1,2-diamine

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The chemistry of the carbon-nitrogen double bond has played a vital role in the progresses of chemistry science. By virtue of both the presence of a lone-pair of electrons on the nitrogen atom and the general electron-donating character of the double bond, compounds containing the azomethine group (Schiff-base compounds) have been used as fine chemicals and medical substrate, as well as ligands coordinating with metal ions in the formation of complexes. Schiff-bases derived from o-hydroxy aromatic aldehydes are of interest due to their ability to show thermo-and photochromic effects which are the consequence of intramolecular proton transfer between oxygen and nitrogen site in the six-membered chelate ring formed by O-H...N (enol-imino or benzenoid tautomer) or N-H... O (keto-amino or quinoid tautomer) strong intramolecular hydrogen bond. Schiff bases are of special interest in the literature; they show thermochromic and photochromic properties, which can be a basis for numerous practical applications. The features responsible for such properties are directly connected with ground state and excited state proton transfer. Theoretical studies on the ways of modification the shape of the potential for the proton transfer seem to have also some practical implications. In this study, N,N-Bis(2-hdroxybenzylidene) phenylen-1,2-diamine was synthesised in good yields by using 2-hydroxy benzaldehyde and 1,2-diaminobenzene in absolute ethanol. In STOE IPDS-II diffractometer system, diffraction data of $C_{20}H_{16}N_2O_2$ was collected with using MoKα X-ray radiation in 293K°. Compound was crystallised on orthorhombic system, space group P 21/c. a = 5.9751A°, b = 16.577A°, c = 16.357A°, V = 1619.8A°^{3}, Z = 4. Data collection and cell refinement: Stoe X-Area. To solve and refine the structure we used the programs SHELXS-97 and SHELXL-97, respectively.