

α,α -Dialkyl- and α -alkyl- α -aryl-substituted cyclic imides, lactams, and acetamides show promising anticonvulsant, anxiolytic, and anesthetic activities. While a number of crystal structures of various α -substituted cyclic imides, lactams, and acetamides were reported, no in-depth comparison of crystal structures and solid-state properties of structurally matched compounds have been carried out so far. In this paper, we report molecular structure and intermolecular interactions of three α,α -diethyl-substituted compounds – 3,3-diethylpyrrolidine-2,5-dione, 3,3-diethylpyrrolidin-2-one, and 2,2-diethylacetamide – in the crystalline phase, as studied using single-crystal X-ray diffraction and IR spectroscopy. We found considerable differences in the patterns of H-bonding and packing of the molecules in crystals. These differences correlate with the compounds' melting points and are of significance to physical pharmacy and formulation development of neuroactive drugs.