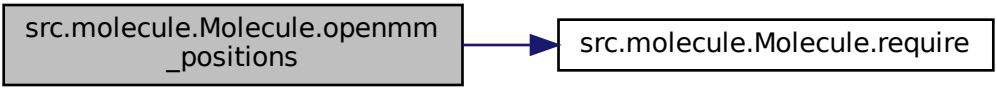
src.molecule.Molecule.openmm
_positions
src.molecule.Molecule.require