

Number	Feature	Dimension
1	One-hot encoding of the atom element	44
2	One-hot encoding of the degree of the atom in the molecule, which is the number of directly-bonded neighbors (atoms)	11
3	One-hot encoding of the total number of H bound to the atom	11
4	One-hot encoding of the number of implicit H bound to the atom	11
5	Whether the atom is aromatic	1
	All	78