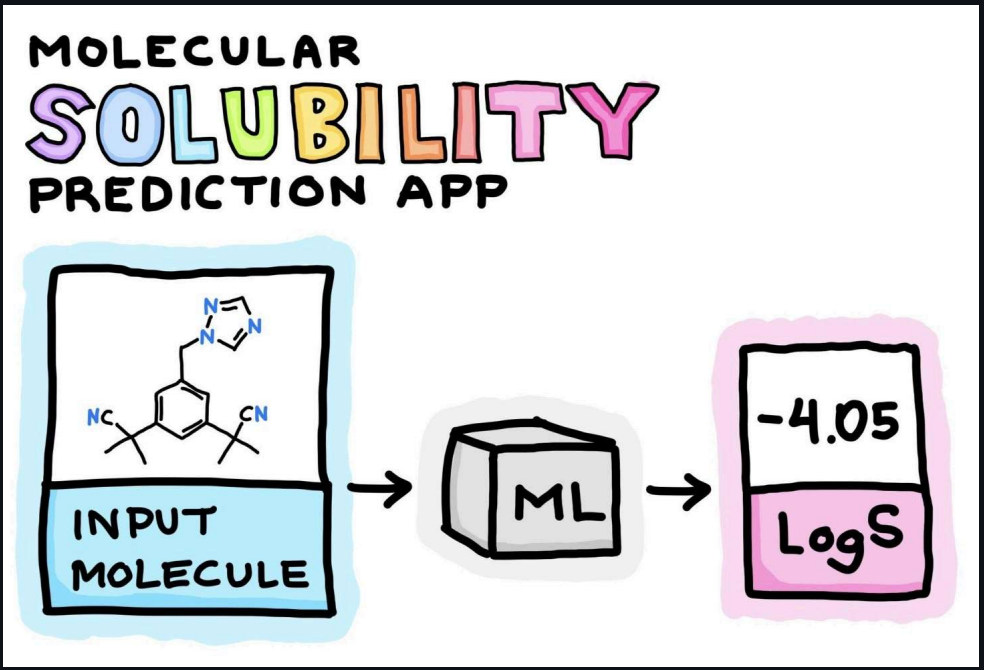
## User Input Features

SMILES input

```
NCCCC
CCC
CN
```




# Molecular Solubility Prediction Web App

This app predicts the **Solubility (LogS)** values of molecules and provides detailed explanations of their structures!

Data obtained from the John S. Delaney. ESOL: Estimating Aqueous Solubility Directly from Molecular Structure. *J. Chem. Inf. Comput. Sci.* 2004, 44, 3, 1000-1005.

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## Input SMILES

```
[
  0 : "NCCCC"
  1 : "CCC"
  2 : "CN"
]
```

## Computed molecular descriptors

| | MolLogP | MolWt | NumRotatableBonds | AromaticProportion |
|---|---|---|---|---|
| 1 | 0.7452 | 73.139 | 2 | 0 |
| 2 | 1.4163 | 44.097 | 0 | 0 |
| 3 | -0.4251 | 31.058 | 0 | 0 |

## Predicted LogS values

| value |
| --- |
| -0.7725 |
| -1.085 |
| 0.3669 |

# Molecular Structure Explanation

Aromatic atoms count: 0

Single bonds count: 2

Double bonds count: 3

Aliphatic atoms count: 0