



Formula: C₆H₆N₂O₂

MW: 138.13

CAS: 104-98-3

MDL:

TNP:



LogP: 1.79

LogS: -4.24

Acceptors: 2

Donors: 2

Rotation Bonds: 2

Chiral Centers: 0

N+O: 4

LIPINSKY: 4

Info: Urocanic acid 99%

IUPAC: (2E)-3-imidazol-4-ylprop-2-enoic acid

Smiles: C(/c1c[nH]cn1)=CC(O)=O

REFERENCE: Urocanic acid was first isolated in 1874 by the chemist M. Jaff