# Cyclooctyne

**Inchi:** InChI=1S/C8H12/c1-2-4-6-8-7-5-3-1/h1-6H2
**InchiKey:** ZPWOOKQUDFIEIX-UHFFFAOYSA-N
**Formula:** C8H12
**SMILES:** C1#CCCCCCC1
**Mol. weight [g/mol]:** 108.18
**CAS:** 1781-78-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ie | 8.90 | eV | NIST Webbook |
| ie | 9.10 | eV | NIST Webbook |
| log10ws | -2.86 | | Crippen Method |
| logp | 2.344 | | Crippen Method |
| mcvol | 104.120 | ml/mol | McGowan Method |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1781788&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

## Legend

**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume