# Phenyl radical

**Inchi:** InChI=1S/C6H5/c1-2-4-6-5-3-1/h1-5H
**InchiKey:** CIUQDSCDWFSTQR-UHFFFAOYSA-N
**Formula:** C6H5
**SMILES:** [c]1ccccc1
**Mol. weight [g/mol]:** 77.10
**CAS:** 2396-01-2

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 884.00 | kJ/mol | NIST Webbook |
| basg | 851.50 | kJ/mol | NIST Webbook |
| ea | 2.17 | eV | NIST Webbook |
| ea | 2.36 ± 0.04 | eV | NIST Webbook |
| ea | 1.20 ± 0.20 | eV | NIST Webbook |
| ea | 1.10 ± 0.01 | eV | NIST Webbook |
| hf | 339.00 ± 8.00 | kJ/mol | NIST Webbook |
| hfpiz | 1149.00 | kJ/mol | NIST Webbook |
| ie | 8.67 ± 0.02 | eV | NIST Webbook |
| ie | 9.20 | eV | NIST Webbook |
| ie | 8.10 ± 0.10 | eV | NIST Webbook |
| ie | 8.32 ± 0.04 | eV | NIST Webbook |
| log10ws | -1.16 | | Crippen Method |
| logp | 1.487 | | Crippen Method |
| mcvol | 69.490 | ml/mol | McGowan Method |

# Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C2396012&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **ea:** | Electron affinity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfpiz:** | Enthalpy of formation of positive ion at 0K |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |