# Cycloheptatrienyl radical

**Inchi:** InChI=1S/C7H7/c1-2-4-6-7-5-3-1/h1-7H
**InchiKey:** WIQYRPSOJMHAHR-UHFFFAOYSA-N
**Formula:** C7H7
**SMILES:** [CH]1C=CC=CC=C1
**Mol. weight [g/mol]:** 91.13
**CAS:** 3551-27-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 832.40 | kJ/mol | NIST Webbook |
| basg | 800.00 | kJ/mol | NIST Webbook |
| ea | 0.49 ± 0.13 | eV | NIST Webbook |
| ea | 0.39 ± 0.04 | eV | NIST Webbook |
| gf | 162.67 | kJ/mol | Joback Method |
| hf | 89.50 | kJ/mol | Joback Method |
| hfus | 8.97 | kJ/mol | Joback Method |
| hvap | 32.51 | kJ/mol | Joback Method |
| ie | 6.24 ± 0.01 | eV | NIST Webbook |
| ie | 6.60 ± 0.10 | eV | NIST Webbook |
| ie | 6.28 ± 0.02 | eV | NIST Webbook |
| ie | 6.24 ± 0.01 | eV | NIST Webbook |
| ie | 6.74 ± 0.05 | eV | NIST Webbook |
| log10ws | -1.82 | | Crippen Method |
| logp | 1.873 | | Crippen Method |
| mcvol | 83.580 | ml/mol | McGowan Method |
| pc | 4397.41 | kPa | Joback Method |
| tb | 380.16 | K | Joback Method |
| tc | 594.48 | K | Joback Method |
| tf | 191.16 | K | Joback Method |
| vc | 0.301 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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|---|---|---|---|---|
| cpg | 129.53 | J/mol×K | 380.16 | Joback Method |
| cpg | 142.11 | J/mol×K | 415.88 | Joback Method |
| cpg | 153.81 | J/mol×K | 451.60 | Joback Method |
| cpg | 164.68 | J/mol×K | 487.32 | Joback Method |
| cpg | 174.76 | J/mol×K | 523.04 | Joback Method |
| cpg | 184.10 | J/mol×K | 558.76 | Joback Method |
| cpg | 192.76 | J/mol×K | 594.48 | Joback Method |
| dvisc | 0.0012422 | Pa×s | 191.16 | Joback Method |
| dvisc | 0.0008172 | Pa×s | 222.66 | Joback Method |
| dvisc | 0.0005964 | Pa×s | 254.16 | Joback Method |
| dvisc | 0.0004666 | Pa×s | 285.66 | Joback Method |
| dvisc | 0.0003833 | Pa×s | 317.16 | Joback Method |
| dvisc | 0.0003262 | Pa×s | 348.66 | Joback Method |
| dvisc | 0.0002852 | Pa×s | 380.16 | Joback Method |

# Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C3551277&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

**affp:** Proton affinity
**basg:** Gas basicity
**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**ea:** Electron affinity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume

| | |
|---|---|
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |