# 1-Heptyl radical

**Inchi:** InChI=1S/C7H15/c1-3-5-7-6-4-2/h1,3-7H2,2H3
**InchiKey:** AQMHNCQZLQUNJI-UHFFFAOYSA-N
**Formula:** C7H15
**SMILES:** [CH2]CCCCCC
**Mol. weight [g/mol]:** 99.19
**CAS:** 3356-67-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 60.44 | kJ/mol | Joback Method |
| hf | -132.00 | kJ/mol | Joback Method |
| hfus | 15.57 | kJ/mol | Joback Method |
| hvap | 31.03 | kJ/mol | Joback Method |
| ie | 7.90 ± 0.06 | eV | NIST Webbook |
| log10ws | -2.36 | | Crippen Method |
| logp | 2.791 | | Crippen Method |
| mcvol | 107.340 | ml/mol | McGowan Method |
| pc | 2934.52 | kPa | Joback Method |
| tb | 358.86 | K | Joback Method |
| tc | 519.50 | K | Joback Method |
| tf | 185.02 | K | Joback Method |
| vc | 0.418 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 188.79 | J/mol×K | 358.86 | Joback Method |
| cpg | 241.05 | J/mol×K | 492.73 | Joback Method |
| cpg | 231.54 | J/mol×K | 465.95 | Joback Method |
| cpg | 221.57 | J/mol×K | 439.18 | Joback Method |
| cpg | 211.14 | J/mol×K | 412.41 | Joback Method |
| cpg | 200.22 | J/mol×K | 385.63 | Joback Method |
| cpg | 250.14 | J/mol×K | 519.50 | Joback Method |
| dvisc | 0.0003092 | Pa×s | 358.86 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003507 | Pa×s | 329.89 | Joback Method |
| dvisc | 0.0004077 | Pa×s | 300.91 | Joback Method |
| dvisc | 0.0004893 | Pa×s | 271.94 | Joback Method |
| dvisc | 0.0006134 | Pa×s | 242.97 | Joback Method |
| dvisc | 0.0008175 | Pa×s | 213.99 | Joback Method |
| dvisc | 0.0011920 | Pa×s | 185.02 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3356670&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |